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\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS	4	OCT 28	KOREAPAT now available on STN
NEWS	5	NOV 30	PHAR reloaded with additional data
NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS	16	JAN 03	No connect-hour charges in EPFULL during January and February 2005
NEWS	17	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	18	FEB 10	STN Patent Forums to be held in March 2005
NEWS	19	FEB 16	STN User Update to be held in conjunction with the 229th ACS National Meeting on March 13, 2005
NEWS	20	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	21	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	22	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	23	MAR 02	GBFULL: New full-text patent database on STN
NEWS	24	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	25	MAR 03	MEDLINE file segment of TOXCENTER reloaded

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.



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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 14:24:27 ON 04 MAR 2005

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE  
ENTRY

TOTAL  
SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 14:24:51 ON 04 MAR 2005

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 MAR 2005 HIGHEST RN 841200-41-7

DICTIONARY FILE UPDATES: 2 MAR 2005 HIGHEST RN 841200-41-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

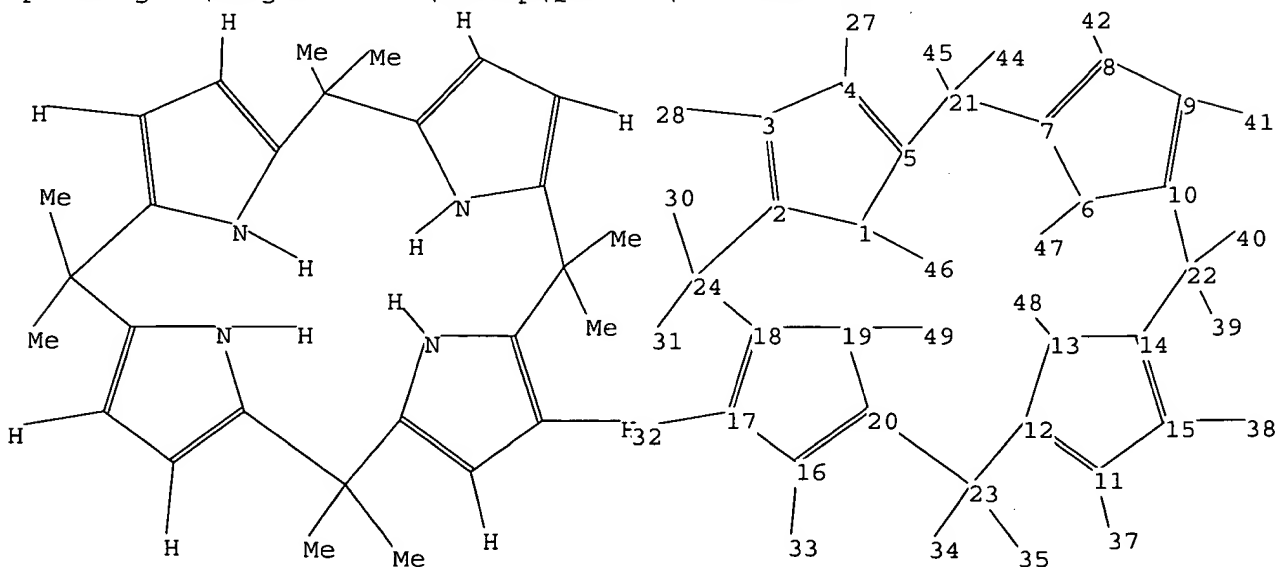
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\09838998c.str



chain nodes :

27 28 30 31 32 33 34 35 37 38 39 40 41 42 44 45 46 47 48 49



```

ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  19  20  21  22  23
24
chain bonds :
1-46  3-28  4-27  6-47  8-42  9-41  11-37  13-48  15-38  16-33  17-32  19-49  21-44
21-45  22-39  22-40  23-34  23-35  24-30  24-31
ring bonds :
1-2  1-5  2-3  2-24  3-4  4-5  5-21  6-7  6-10  7-8  7-21  8-9  9-10  10-22  11-12
11-15  12-13  12-23  13-14  14-15  14-22  16-17  16-20  17-18  18-19  18-24  19-20
20-23
exact/norm bonds :
1-2  1-5  2-3  2-24  3-4  4-5  5-21  6-7  6-10  7-8  7-21  8-9  9-10  10-22  11-12
11-15  12-13  12-23  13-14  14-15  14-22  16-17  16-20  17-18  18-19  18-24  19-20
20-23
exact bonds :
1-46  3-28  4-27  6-47  8-42  9-41  11-37  13-48  15-38  16-33  17-32  19-49  21-44
21-45  22-39  22-40  23-34  23-35  24-30  24-31
isolated ring systems :
containing 1 :

```

G1:C,H,X,Ak,OH

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 27:CLASS 28:CLASS 30:CLASS 31:CLASS
32:CLASS 33:CLASS 34:CLASS 35:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS
41:CLASS 42:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS

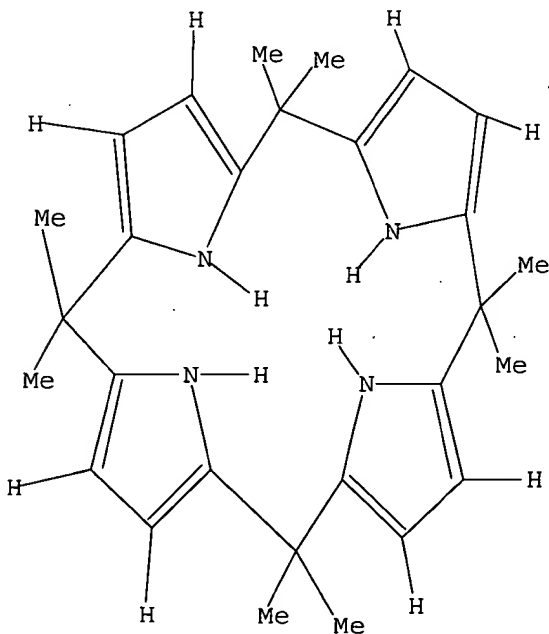
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L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 C,H,X,Ak,OH



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 14:25:11 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 2143 TO ITERATE

100.0% PROCESSED 2143 ITERATIONS 30 ANSWERS  
SEARCH TIME: 00.00.01

L2 30 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	161.54

FILE 'CAPLUS' ENTERED AT 14:25:13 ON 04 MAR 2005  
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FILE COVERS 1907 - 4 Mar 2005 VOL 142 ISS 11  
FILE LAST UPDATED: 3 Mar 2005 (20050303/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l2

L3 66 L2

=> s l3 and complexing agent

39820 COMPLEXING  
718437 AGENT  
1025234 AGENTS  
1453810 AGENT  
(AGENT OR AGENTS)  
16359 COMPLEXING AGENT  
(COMPLEXING(W)AGENT)  
L4 1 L3 AND COMPLEXING AGENT

=> d ibib abs hitstr

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2003:827065 CAPLUS  
DOCUMENT NUMBER: 140:16713  
TITLE: Calix[2]bipyrrole[2]furan and  
Calix[2]bipyrrole[2]thiophene: New Pyrrolic Receptors  
Exhibiting a Preference for Carboxylate Anions  
AUTHOR(S): Sessler, Jonathan L.; An, Deqiang; Cho, Won-Seob;  
Lynch, Vincent



CORPORATE SOURCE: Department of Chemistry and Biochemistry, Institute for Cellular and Molecular Biology, The University of Texas at Austin, Austin, TX, 78712-0165, USA

SOURCE: Journal of the American Chemical Society (2003), 125(45), 13646-13647  
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

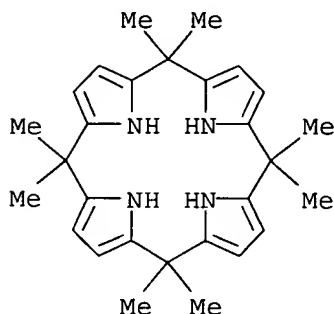
OTHER SOURCE(S): CASREACT 140:16713

AB Heterocycles other than pyrrole, specifically bipyrrrole, furan, and thiophene, have been used to construct two new, calixpyrrole-like anion receptors; binding studies, carried out by isothermal titration calorimetry (ITC) in CH<sub>3</sub>CN, reveal a selectivity for Y-shaped anions, such as benzoate, over spherical ones, such as chloride. The binding consts. of these new anion receptors were compared to 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine, 6,6,15,15,24,24-hexamethyl-28,29,30,31,32,33-Hexaazaheptacyclo[23.2.1.12,5.17,10.111,14.116,19.120,23]tritriaconta-2,4,7,9,11,13,16,18,20,22,25,27-dodecaene, etc.

IT 4475-42-7  
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
(preparation of calix[2]bipyrrrole[2]furan and calix[2]bipyrrrole[2]thiophene; pyrrolic receptors exhibiting preference for carboxylate anions)

RN 4475-42-7 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s 13 and anion binding  
200185 ANION  
107720 ANIONS  
265434 ANION  
(ANION OR ANIONS)  
856548 BINDING  
1886 BINDINGS  
857077 BINDING  
(BINDING OR BINDINGS)  
1743 ANION BINDING  
(ANION(W)BINDING)  
L5 14 L3 AND ANION BINDING

=> s 15 and tetrabutylammonium chloride  
20957 TETRABUTYLAMMONIUM  
1020760 CHLORIDE  
151577 CHLORIDES  
1089863 CHLORIDE  
(CHLORIDE OR CHLORIDES)



1785 TETRABUTYLAMMONIUM CHLORIDE  
(TETRABUTYLAMMONIUM(W) CHLORIDE)

L6 4 L5 AND TETRABUTYLAMMONIUM CHLORIDE

=> d ibib abs hitstr l6 1-4

L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:385522 CAPLUS

DOCUMENT NUMBER: 139:100832

TITLE: Single Side Strapping: A New Approach to Fine Tuning  
the Anion Recognition Properties of Calix[4]pyrroles

AUTHOR(S): Lee, Chang-Hee; Na, Hee-Kyung; Yoon, Dae-Wi; Won,  
Dong-Hoon; Cho, Won-Seob; Lynch, Vincent M.; Shevchuk,  
Sergey V.; Sessler, Jonathan L.

CORPORATE SOURCE: Department of Chemistry, Kangwon National University,  
Chun-Chon, 200-701, S. Korea

SOURCE: Journal of the American Chemical Society (2003),  
125(24), 7301-7306

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:100832

AB Three calix[4]pyrroles bearing m-orcinol-derived diether straps of  
different lengths on one side of the tetrapyrrolic core were synthesized  
and characterized. Structural information for an analogous diester  
bridged strapped system reported previously (Yoon, D. W.; Hwang, H.; Lee,  
C. H. Angew. Chemical, Int. Ed. Engl. 2002, 41, 1757-1759) is also provided  
as are bromide and chloride anion affinities for all four systems determined by  
Isothermal Titration Calorimetry (ITC) in acetonitrile. Although both sets  
of the strapped calix[4]pyrroles displayed enhanced affinities for  
chloride and bromide anion, differences were seen among the various  
receptors that support the conclusion that the **anion**  
**binding** ability of calixpyrrole-type systems can be effectively  
tuned by modifying the length and nature of the bridging straps. In the  
specific case of the diether systems, the largest chloride affinity was  
seen with the shortest strap, whereas the largest affinity for bromide  
anion was recorded in the case of the longest strap. As well as  
supporting 1H NMR spectroscopic studies, it is postulated that not only  
cavity size per se, but also the ability of the aryl portion of the strap  
to serve as a CH H bond donor site are important in regulating the observed  
anion affinities.

IT 4475-42-7

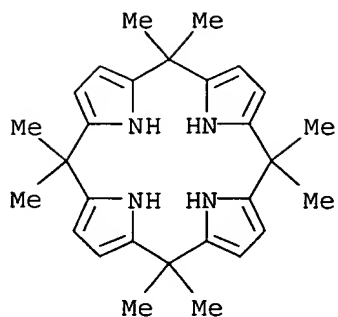
RL: CPS (Chemical process); PEP (Physical, engineering or chemical  
process); PRP (Properties); PYP (Physical process); RCT (Reactant); PROC  
(Process); RACT (Reactant or reagent)

(complexation of halide salts; single side strapping approach to fine  
tuning anion recognition properties of calix[4]pyrroles)

RN 4475-42-7 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-  
octamethyl- (9CI) (CA INDEX NAME)





IT 311804-85-0 560094-15-7 560094-20-4

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); FORM (Formation, nonpreparative); PROC (Process)

(single side strapping approach to fine tuning anion recognition properties of calix[4]pyrroles)

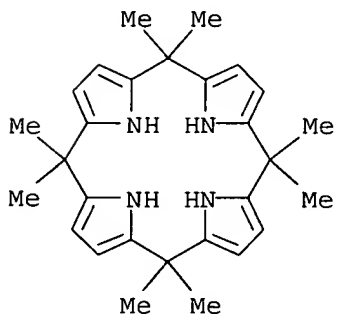
RN 311804-85-0 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, chloride, compd. with 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 4475-42-7

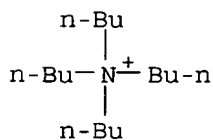
CMF C28 H36 N4



CM 2

CRN 1112-67-0

CMF C16 H36 N . Cl



● Cl<sup>-</sup>

RN 560094-15-7 CAPLUS

CN Potassium(1+), (4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane-



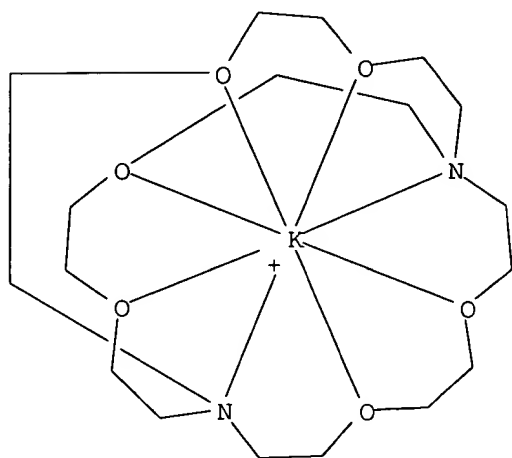
$\kappa N1, \kappa N10, \kappa O4, \kappa O7, \kappa O13, \kappa O16, \kappa O21, \kappa O24$ )-, chloride, compd. with 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 12569-48-1

CMF C18 H36 K N2 O6 . Cl

CCI CCS

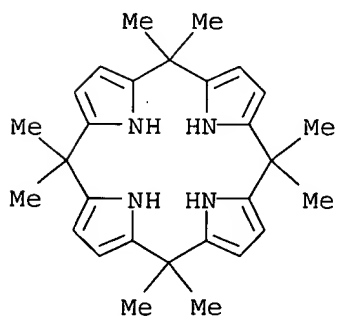


● Cl -

CM 2

CRN 4475-42-7

CMF C28 H36 N4



RN 560094-20-4 CAPLUS

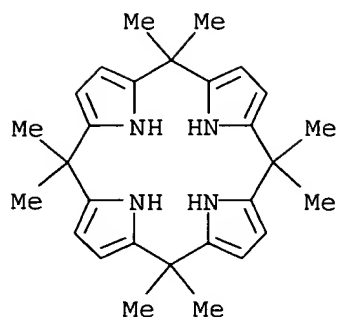
CN 1-Butanaminium, N,N,N-tributyl-, bromide, compd. with 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 4475-42-7

CMF C28 H36 N4

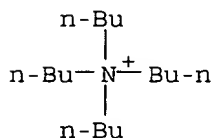




CM 2

CRN 1643-19-2

CMF C16 H36 N . Br



● Br<sup>-</sup>

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:593350 CAPLUS

DOCUMENT NUMBER: 138:73246

TITLE: Mono halogen substituted calix[4]pyrroles: fine-tuning the **anion binding** properties of calix[4]pyrrole

AUTHOR(S): Miyaji, Hidekazu; An, Deqiang; Sessler, Jonathan L.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, University of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Supramolecular Chemistry (2001), 13(6), 661-669  
CODEN: SCHEER; ISSN: 1061-0278

PUBLISHER: Gordon & Breach Science Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Single halogen atom (i.e. I, Br, Cl and F) substituted calix[4]pyrroles, compds. were synthesized. Studies of these systems reveal that replacement of a single  $\beta$ -pyrrolic hydrogen atom can increase the **anion binding** ability of calix[4]pyrroles for a variety of anions (e.g. Cl<sup>-</sup>, Br<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup> and HSO<sub>4</sub><sup>-</sup>) relative to normal non-halogen substituted calix[4]pyrrole. In the case of chloride anion, the expected relative affinity sequence of for these compds. was observed This was not found to be true for Br<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, and HSO<sub>4</sub><sup>-</sup>. Here, the chlorine substituted calix[4]pyrrole was found to display a slightly higher affinity in the case of each anion than the fluorine-bearing derivative This was rationalized in terms of intermol. NH...F hydrogen bonding interactions being present in CD<sub>2</sub>Cl<sub>2</sub> solns. of fluorine compound Support for this latter conclusion came from concentration and temperature-dependent

NMR



spectroscopic studies. A matched set of mono halogen substituted calix[4]pyrroles was used to study in detail, the extent to which halogen substituents may be used to fine-tune the **anion binding** properties of calix[4]pyrroles.

IT 4475-42-7

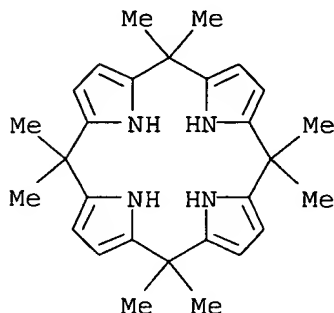
RL: RCT (Reactant); RACT (Reactant or reagent)

(halogenation of; preparation and anion binding

properties of monohalogen-substituted calix[4]pyrroles)

RN 4475-42-7 CAPLUS

CN	21H,23H-Porphine, 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-	(9CI)	(CA INDEX NAME)
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REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:570756 CAPLUS

DOCUMENT NUMBER: 133:321732

TITLE: Modified Calix[4]pyrroles

AUTHOR(S) : Sessler, Jonathan L.; Anzenbacher, Pavel, Jr.; Miyaji, Hidekazu; Jursikova, Karolina; Bleasdale, Ellen R.; Gale, Philip A.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute  
for Cellular and Molecular Biology, University of  
Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Industrial & Engineering Chemistry Research (2000), 39(10), 3471-3478

CODEN: IECRED; ISSN: 0888-5885

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S) : CASREACT 133:321732

AB The synthesis and chemical properties of a variety of chemical modified calix[4]pyrroles were described. The effects of structural changes, specifically the presence and absence of substituents on the meso-like and  $\beta$ -pyrrolic carbons, on anion affinities were detailed as was their effect on macrocycle conformation. Also described were unsym. systems, bearing an aliphatic and aromatic substituent on each of the four meso-like carbon atoms. In this case, the properties of the resulting configuration isomers are discussed in terms, again, of the resulting effects on macrocycle conformation and substrate binding affinity. Finally, the use of appropriately functionalized calix[4]pyrrole systems as rudimentary fluorescence-based anion sensors is presented.

IT 4475-42-7

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)

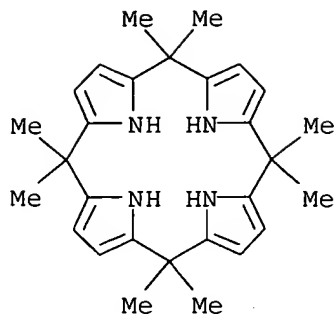
```
(preparation, anion binding affinity, and conformation
```

of modified calix[4]pyrroles)

RN 4475-42-7 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:288186 CAPLUS

DOCUMENT NUMBER: 125:33102

TITLE: Calix[4]pyrroles: Old Yet New **Anion-Binding** Agents

AUTHOR(S): Gale, Philip A.; Sessler, Jonathan L.; Kral, Vladimir; Lynch, Vincent

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Texas, Austin, TX, 78712-1167, USA

SOURCE: Journal of the American Chemical Society (1996), 118(21), 5140-5141

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The octaalkylporphyrinogens, octamethylcalix[4]pyrrole [i.e., 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine,] (I) and tetraspirocyclohexylcalix[4]pyrrole (II), have been found to be effective **anion binding** agents both in solution and in the solid state. Evidence for **anion binding** in the solid state derives from single crystal x-ray diffraction analyses with structures of the chloride complex of I and the fluoride complex of II being explicitly obtained. In these structures, the calix[4]pyrrole ligands are found in cone-like conformations such that the pyrrole NH protons can coordinate to the bound halide anions via hydrogen bonds. By contrast, x-ray structural analyses of the free receptors show that, in the absence of anions, compds. I and II adopt 1,3-alternate conformations in the solid state. Proton NMR titration studies, carried out in dichloromethane-d<sub>2</sub> solution, reveal that both compound are selective for fluoride over a variety of other anions (viz, Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup> and HSO<sub>4</sub><sup>-</sup>).

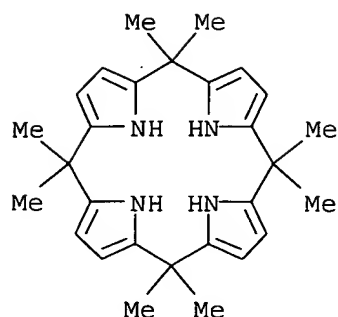
IT 4475-42-7

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
(complexation behavior of calix[4]pyrroles (porphines) with anions)

RN 4475-42-7 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)





IT 177570-04-6P 177695-35-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(complexation behavior of calix[4]pyrroles (porphines) with anions)

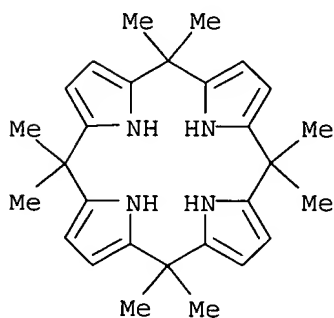
RN 177570-04-6 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, chloride, compd. with dichloromethane and  
stereoisomer of 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-  
octamethyl-21H,23H-porphine (1:1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177570-03-5

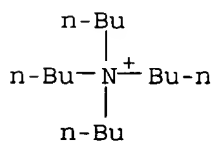
CMF C28 H36 N4



CM 2

CRN 1112-67-0

CMF C16 H36 N . Cl



● Cl<sup>-</sup>

CM 3

CRN 75-09-2

CMF C H2 Cl2



Cl-CH<sub>2</sub>-Cl

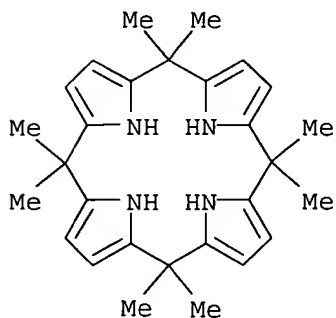
RN 177695-35-1 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, chloride, compd. with stereoisomer of  
5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-  
porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177570-03-5

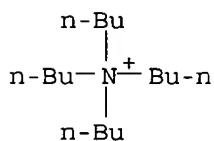
CMF C28 H36 N4



CM 2

CRN 1112-67-0

CMF C16 H36 N . Cl



● Cl<sup>-</sup>

=> d his

(FILE 'HOME' ENTERED AT 14:24:27 ON 04 MAR 2005)

FILE 'REGISTRY' ENTERED AT 14:24:51 ON 04 MAR 2005

L1 STRUCTURE UPLOADED

L2 30 S L1 FULL

FILE 'CAPLUS' ENTERED AT 14:25:13 ON 04 MAR 2005

L3 66 S L2

L4 1 S L3 AND COMPLEXING AGENT

L5 14 S L3 AND ANION BINDING

L6 4 S L5 AND TETRABUTYLAMMONIUM CHLORIDE

=> s l3 and tetrabutylammonium chloride



20957 TETRABUTYLAMMONIUM  
1020760 CHLORIDE  
151577 CHLORIDES  
1089863 CHLORIDE

(CHLORIDE OR CHLORIDES)

1785 TETRABUTYLAMMONIUM CHLORIDE  
(TETRABUTYLAMMONIUM(W) CHLORIDE)

L7 5 L3 AND TETRABUTYLAMMONIUM CHLORIDE

=> s l7 not l6

L8 1 L7 NOT L6

=> d ibib abs hitstr

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:497540 CAPLUS

DOCUMENT NUMBER: 139:245635

TITLE: Selective recognition of halide anions by  
calix[4]pyrrole: a detailed thermodynamic study

AUTHOR(S): Danil De Namor, Angela F.; Shehab, Mohammed

CORPORATE SOURCE: Laboratory of Thermochemistrn, Department of  
Chemistry, University of Surrey, Surrey, GU2 7XH, UK

SOURCE: Journal of Physical Chemistry B (2003), 107(26),  
6462-6468

CODEN: JPCBFK; ISSN: 1520-6106

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Several anal. techniques (1H NMR, conductance measurements, and titration calorimetry) were used to assess the interaction of calix[4]pyrrole and halide anions in dipolar aprotic solvents (acetonitrile and N,N-dimethylformamide). Solubility data for calix[4]pyrrole in various solvents at 298.15 K were determined. These data were used to calculate the standard

Gibbs energies of solution. Taking acetonitrile as the reference solvent, the transfer Gibbs energies of this ligand to various solvents were calculated. Chemical shift changes ( $\Delta\delta$ ) of the pyrrole proton relative to the free ligand resulting from the addition of the anion salts to the ligand in CD<sub>3</sub>CN at 298 K follow the sequence F<sup>-</sup> > Cl<sup>-</sup> > Br<sup>-</sup> > I<sup>-</sup>. Conductance measurements were performed (i) to establish the stoichiometry of the anionic calix[4]pyrrole complexes and (ii) to assess the range of concentration at which the free and complex anion salts are predominantly in their ionic forms in acetonitrile and N,N-dimethylformamide at 298.15 K. Titration calorimetry was used to determine the stability constant, K<sub>s</sub>, (hence the standard

Gibbs energy) and the enthalpy. Combination of Gibbs energy and enthalpy data yields the entropy of complexation. A linear correlation is found between the log K<sub>s</sub> and the  $\Delta\delta$  values. Calix[4]pyrrole is able to recognize selectively the halide anions in these solvents. The selectivity of the ligand for one anion relative to another is quant. evaluated through the calcn. of the selectivity factor. The ligand behavior is representative of flexible ligands in which calix[4]pyrrole compete successfully with the solvent for the anion to an extent that the higher selectivity of the ligand is for the smallest anion (fluoride). The thermodyn. of complexation is discussed in terms of the solvation properties of the reactants and the products in acetonitrile and N,N-dimethylformamide.

IT 240799-02-4 240799-03-5 240799-04-6  
240799-05-7 311804-84-9 311804-85-0  
560094-20-4

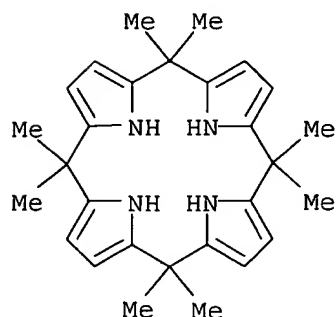
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)



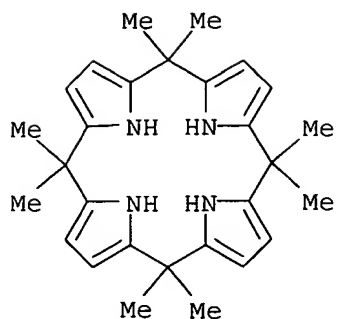
(thermodn. study of selective recognition of halide anions by  
calix[4]pyrrole)

RN 240799-02-4 CAPLUS

CN Fluoride, compd. with 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)



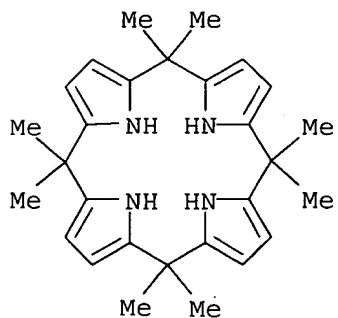




● Br<sup>-</sup>

RN 240799-05-7 CAPLUS

CN Iodide, compd. with 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)



● I<sup>-</sup>

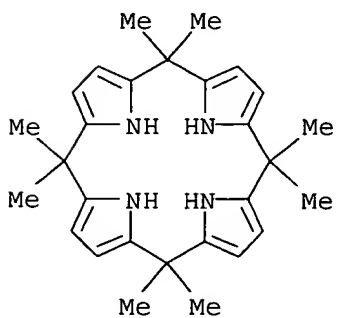
RN 311804-84-9 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, fluoride, compd. with 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 4475-42-7

CMF C28 H36 N4

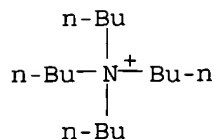




CM 2

CRN 429-41-4

CMF C16 H36 N . F



● F<sup>-</sup>

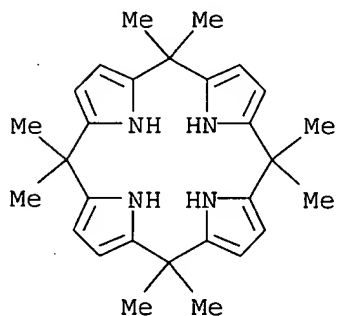
RN 311804-85-0 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, chloride, compd. with  
5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-  
porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 4475-42-7

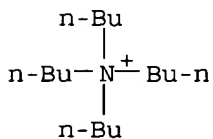
CMF C28 H36 N4



CM 2

CRN 1112-67-0

CMF C16 H36 N . Cl



● Cl<sup>-</sup>

RN 560094-20-4 CAPLUS

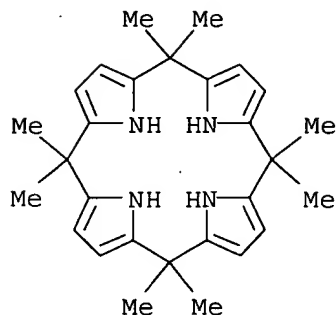
CN 1-Butanaminium, N,N,N-tributyl-, bromide, compd. with 5,10,15,20,22,24-  
hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI)  
(CA INDEX NAME)



CM 1

CRN 4475-42-7

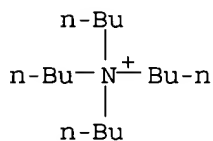
CMF C28 H36 N4



CM 2

CRN 1643-19-2

CMF C16 H36 N . Br



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

48.36

209.90

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-4.38

-4.38

FILE 'REGISTRY' ENTERED AT 14:30:03 ON 04 MAR 2005

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STRUCTURE FILE UPDATES: 2 MAR 2005 HIGHEST RN 841200-41-7

DICTIONARY FILE UPDATES: 2 MAR 2005 HIGHEST RN 841200-41-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005



Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

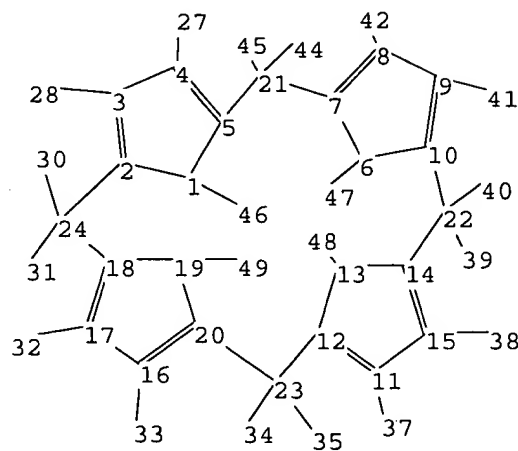
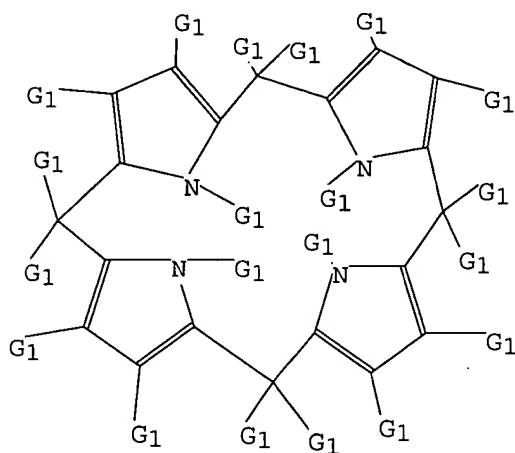
Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\09838998y.str

X

51



chain nodes :

27 28 30 31 32 33 34 35 37 38 39 40 41 42 44 45 46 47 48 49 51

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23  
24

chain bonds :

1-46 3-28 4-27 6-47 8-42 9-41 11-37 13-48 15-38 16-33 17-32 19-49 21-44  
21-45 22-39 22-40 23-34 23-35 24-30 24-31

ring bonds :

1-2 1-5 2-3 2-24 3-4 4-5 5-21 6-7 6-10 7-8 7-21 8-9 9-10 10-22 11-12  
11-15 12-13 12-23 13-14 14-15 14-22 16-17 16-20 17-18 18-19 18-24 19-20  
20-23

exact/norm bonds :

1-2 1-5 1-46 2-3 2-24 3-4 3-28 4-5 4-27 5-21 6-7 6-10 6-47 7-8 7-21  
8-9 8-42 9-10 9-41 10-22 11-12 11-15 11-37 12-13 12-23 13-14 13-48  
14-15 14-22 15-38 16-17 16-20 16-33 17-18 17-32 18-19 18-24 19-20 19-49  
20-23 21-44 21-45 22-39 22-40 23-34 23-35 24-30 24-31



isolated ring systems :  
containing 1 :

G1:C,H,X,Ak,OH

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom  
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 27:CLASS 28:CLASS 30:CLASS 31:CLASS  
32:CLASS 33:CLASS 34:CLASS 35:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS  
41:CLASS 42:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS  
51:CLASS

L9 STRUCTURE UPLOADED

=> d

L9 HAS NO ANSWERS

L9 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s 19

SAMPLE SEARCH INITIATED 14:30:22 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1811 TO ITERATE

55.2% PROCESSED 1000 ITERATIONS ( 3 INCOMPLETE) 3 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 33668 TO 38772  
PROJECTED ANSWERS: 3 TO 247

L10 3 SEA SSS SAM L9

=> s 19 full

FULL SEARCH INITIATED 14:30:26 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 37042 TO ITERATE

100.0% PROCESSED 37042 ITERATIONS ( 15 INCOMPLETE) 23 ANSWERS  
SEARCH TIME: 00.00.02

L11 23 SEA SSS FUL L9

=> s 111 and caplus/lc

44463264 CAPLUS/LC

L12 23 L11 AND CAPLUS/LC

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
165.93	375.83

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-4.38

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FILE COVERS 1907 - 4 Mar 2005 VOL 142 ISS 11  
FILE LAST UPDATED: 3 Mar 2005 (20050303/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 112

L13 18 L12

=> d ibib abs hitstr 1-18

L13 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:497321 CAPLUS

DOCUMENT NUMBER: 141:324726

TITLE: Optical anion sensors based on alkyne-linked, functionalized calix[4]pyrroles

AUTHOR(S): Miyaji, Hidekazu; Sato, Wataru; An, Deqiang; Sessler, Jonathan L.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, The University of Texas at Austin, Austin, TX, 78712-0165, USA

SOURCE: Collection of Czechoslovak Chemical Communications (2004), 69(5), 1027-1049

CODEN: CCCCAK; ISSN: 0010-0765

PUBLISHER: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Linking a calix[4]pyrrole anion recognition subunit to chromophores or fluorophores via an alkynyl spacer attached to a  $\beta$ -pyrrolic position of a calix[4]pyrrole core produces a new class of anion sensor that permits the detection of halide and phosphate anions in organic media via direct, so-called naked-eye visualization or fluorescence quenching-based spectroscopic means.

IT 265137-00-6P

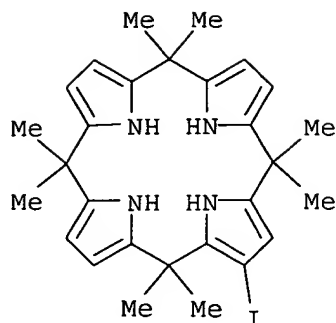
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(anions determination by optical sensors based on alkyne-linked, functionalized calix[4]pyrroles)

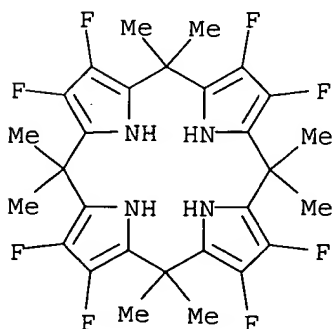
RN 265137-00-6 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20,22,24-hexahydro-2-iodo-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)





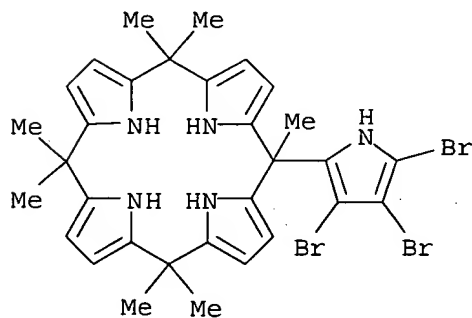
L13 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2003:623230 CAPLUS  
 DOCUMENT NUMBER: 139:370552  
 TITLE: Fluorinated calixpyrroles: anion-binding extractants that reduce the Hofmeister bias  
 AUTHOR(S): Levitskaia, Tatiana G.; Marquez, Manuel; Sessler, Jonathan L.; Shriver, James A.; Vercouter, Thomas; Moyer, Bruce A.  
 CORPORATE SOURCE: Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37830-6119, USA  
 SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (17), 2248-2249  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB  $\beta$ -Octafluoro-meso-octamethylcalix[4]pyrrole (I) and  $\beta$ -decafluoro-meso-decamethylcalix[5]pyrrole (II) were found to extract cesium salts of smaller anions (bromide and chloride for I and nitrate for II) as effectively as that of iodide into nitrobenzene (NB) thereby overcoming the Hofmeister bias normally observed for processes of this type.  
 IT **311804-81-6**  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)  
 (cesium salt solvent extn with fluorinated calixpyrroles and attenuation of Hofmeister series)  
 RN 311804-81-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

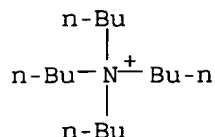


ACCESSION NUMBER: 2003:534192 CAPLUS  
 DOCUMENT NUMBER: 140:42149  
 TITLE: Pentapyrrolic calix[4]pyrrole  
 AUTHOR(S): Warriner, Colin N.; Gale, Philip A.; Light, Mark E.;  
 Hursthouse, Michael B.  
 CORPORATE SOURCE: School of Chemistry, University of Southampton,  
 Southampton, SO17 1BJ, UK  
 SOURCE: Chemical Communications (Cambridge, United Kingdom)  
 (2003), (15), 1810-1811  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 140:42149  
 AB A new calix[4]pyrrole has been synthesized that contains a  
 3,4,5-trisbromopyrrole appended to a meso-position. This compound shows  
 enhanced anion affinity as compared to the parent meso-  
 octamethylcalix[4]pyrrole macrocycle. Crystal structure of the  
 intermediate and mol. modeling of the product were also investigated.  
 IT **634892-93-6**  
 RL: PRP (Properties)  
 (conformation of acetate-pentapyrrolic calix[4]pyrrole complex studied  
 via mol. modeling)  
 RN 634892-93-6 CAPLUS  
 CN 1-Butanaminium, N,N,N-tributyl-, acetate, compd. with 5,10,15,20,22,24-  
 hexahydro-5,5,10,10,15,15,20-heptamethyl-20-(3,4,5-tribromo-1H-pyrrol-2-  
 yl)-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 634892-91-4  
 CMF C31 H34 Br3 N5



CM 2  
 CRN 10534-59-5  
 CMF C16 H36 N . C2 H3 O2  
 CM 3  
 CRN 10549-76-5  
 CMF C16 H36 N

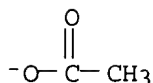




CM 4

CRN 71-50-1

CMF C2 H3 O2

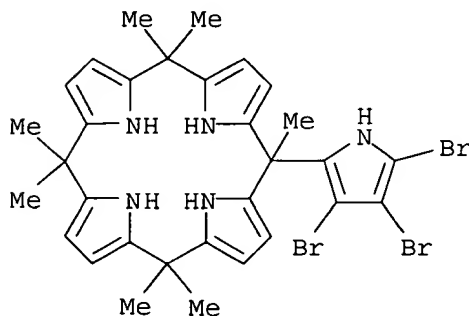


IT 634892-91-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation, enhanced anion affinity, and mol. modeling of pentapyrrolic  
calix[4]pyrrole)

RN 634892-91-4 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20-  
heptamethyl-20-(3,4,5-tribromo-1H-pyrrol-2-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:385522 CAPLUS

DOCUMENT NUMBER: 139:100832

TITLE: Single Side Strapping: A New Approach to Fine Tuning  
the Anion Recognition Properties of Calix[4]pyrroles

AUTHOR(S): Lee, Chang-Hee; Na, Hee-Kyung; Yoon, Dae-Wi; Won,  
Dong-Hoon; Cho, Won-Seob; Lynch, Vincent M.; Shevchuk,  
Sergey V.; Sessler, Jonathan L.

CORPORATE SOURCE: Department of Chemistry, Kangwon National University,  
Chun-Chon, 200-701, S. Korea

SOURCE: Journal of the American Chemical Society (2003),  
125(24), 7301-7306

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:100832

AB Three calix[4]pyrroles bearing m-orscinol-derived diether straps of  
different lengths on one side of the tetrapyrrolic core were synthesized



and characterized. Structural information for an analogous diester bridged strapped system reported previously (Yoon, D. W.; Hwang, H.; Lee, C. H. *Angew. Chemical, Int. Ed. Engl.* 2002, 41, 1757-1759) is also provided as are bromide and chloride anion affinities for all four systems determined by Isothermal Titration Calorimetry (ITC) in acetonitrile. Although both sets of the strapped calix[4]pyrroles displayed enhanced affinities for chloride and bromide anion, differences were seen among the various receptors that support the conclusion that the anion binding ability of calixpyrrole-type systems can be effectively tuned by modifying the length and nature of the bridging straps. In the specific case of the diether systems, the largest chloride affinity was seen with the shortest strap, whereas the largest affinity for bromide anion was recorded in the case of the longest strap. As well as supporting <sup>1</sup>H NMR spectroscopic studies, it is postulated that not only cavity size per se, but also the ability of the aryl portion of the strap to serve as a CH H bond donor site are important in regulating the observed anion affinities.

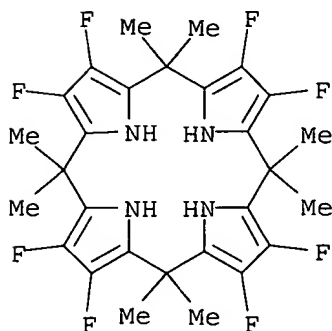
IT 311804-81-6

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(complexation of halide salts; single side strapping approach to fine tuning anion recognition properties of calix[4]pyrroles)

RN 311804-81-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



IT 311804-88-3 560094-16-8 560094-21-5

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); FORM (Formation, nonpreparative); PROC (Process)

(single side strapping approach to fine tuning anion recognition properties of calix[4]pyrroles)

RN 311804-88-3 CAPLUS

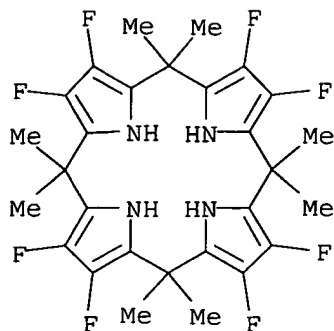
CN 1-Butanaminium, N,N,N-tributyl-, chloride, compd. with 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 311804-81-6

CMF C28 H28 F8 N4

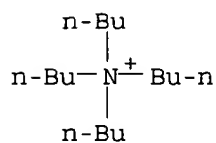




CM 2

CRN 1112-67-0

CMF C16 H36 N . Cl



● Cl -

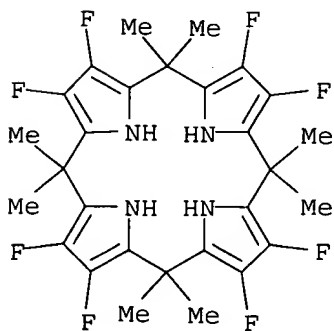
RN 560094-16-8 CAPLUS

CN Potassium(1+), (4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane-  
κN1,κN10,κO4,κO7,κO13,κO16,κO21,  
κO24)-, chloride, compd. with 2,3,7,8,12,13,17,18-octafluoro-  
5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-  
porphine (1:1) (9Cl) (CA INDEX NAME)

CM 1

CRN 311804-81-6

CMF C28 H28 F8 N4

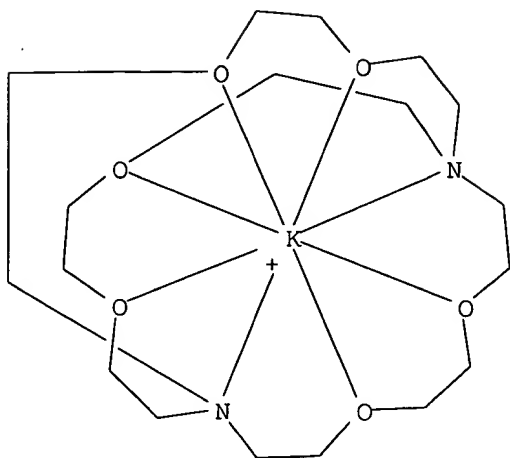


CM 2

CRN 12569-48-1



CMF C18 H36 K N2 O6 . Cl  
 CCI CCS

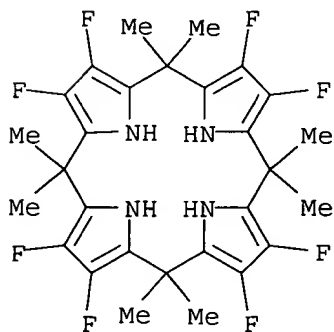


● Cl<sup>-</sup>

RN 560094-21-5 CAPLUS  
 CN 1-Butanaminium, N,N,N-tributyl-, bromide, compd. with 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

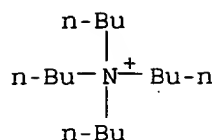
CRN 311804-81-6  
 CMF C28 H28 F8 N4



CM 2

CRN 1643-19-2  
 CMF C16 H36 N . Br





● Br<sup>-</sup>

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:751572 CAPLUS

DOCUMENT NUMBER: 137:389723

TITLE: Theoretical Study of Anion Binding to Calix[4]pyrrole: the Effects of Solvent, Fluorine Substitution, Cosolute, and Water Traces

AUTHOR(S): Blas, J. Ramon; Marquez, Manuel; Sessler, Jonathan L.; Luque, F. Javier; Orozco, Modesto

CORPORATE SOURCE: Departament de Bioquímica i Biologia Molecular, Facultat de Química, Universitat de Barcelona, Barcelona, 08028, Spain

SOURCE: Journal of the American Chemical Society (2002), 124(43), 12796-12805

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The binding of different anions to calix[4]pyrrole has been studied by means of mol. dynamics coupled to thermodyn. integration calcns. The effect of different apolar solvents, octafluoro substitution, and the change in binding free energy derived from the presence of cosolute and water traces (the hydrated salt used to introduce the anion in the solution) were examined. Calcns. allow us to rationalize the differential binding of ions to calix[4]pyrrole and octafluorocalix[4]pyrrole as well as to predict the behavior in new solvents for which exptl. data are not available yet. It is found that both calix[4]pyrrole and octafluorocalix[4]pyrrole have a dramatic preference for F<sup>-</sup> in the gas phase and pure aprotic solvents, but the situation can change dramatically in protic solvents or in the presence of the hydrated cation which is used as cosolute of the anion. Overall, our results provide interesting clues for a better understanding of the process detected exptl. as "binding".

IT 311804-81-6

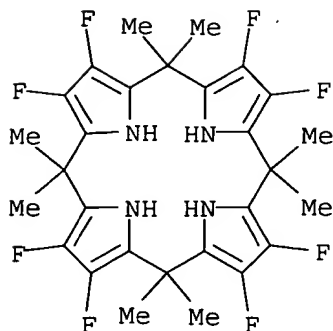
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)

(effects of solvents and fluorine substitution on anion binding to calix[4]pyrrole from mol. dynamics and thermodyn. integration)

RN 311804-81-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)





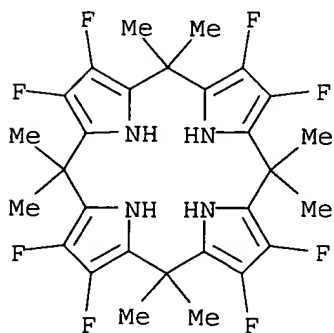
IT 475644-56-5

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(optimized mol. structure of chloride-octafluorocalix[4]pyrrole, fluoride-calix[4]pyrrole, phosphate-calix[4]pyrrol, and fluoride-tetrabutylammonium trihydrate complexes)

RN 475644-56-5 CAPLUS

CN Chloride, compd. with 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:638268 CAPLUS

DOCUMENT NUMBER: 137:185360

TITLE: Preparation, binding properties, and uses of halogenated calixpyrroles, calixpyridinopyrroles and calixpyridines

INVENTOR(S): Sessler, Jonathan L.; Marquez, Manuel; Anzenbacher, Pavel; Shriver, James A.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 104 pp., Cont.-in-part of U.S. Ser. No. 838,998.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:



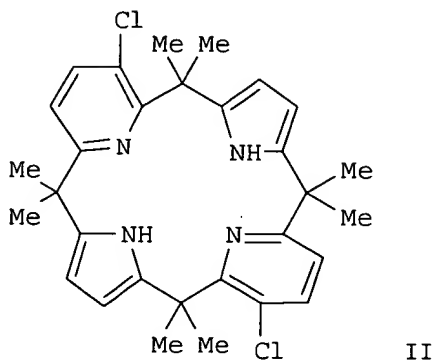
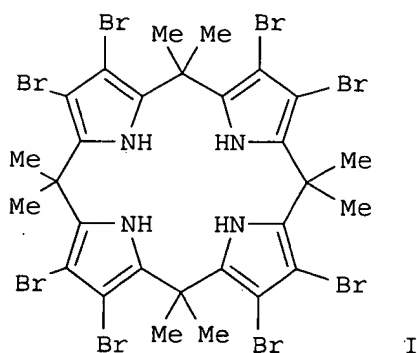
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002115566	A1	20020822	US 2001-939514	20010824
CA 2391030	AA	19971016	CA 1997-2391030	19970404
US 6262257	B1	20010717	US 1997-833379	19970404
US 2002026047	A1	20020228	US 2001-838998	20010420
WO 2003018548	A2	20030306	WO 2002-US27252	20020826
WO 2003018548	A3	20030703		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:  
 US 1996-14890P P 19960405  
 US 1996-24203P P 19960827  
 US 1996-26694P P 19960925  
 US 1996-33395P P 19961217  
 US 1996-33396P P 19961217  
 US 1997-833379 A3 19970404  
 US 2001-838998 A2 20010420  
 CA 1997-2251072 A3 19970404  
 US 2001-939514 A 20010824

OTHER SOURCE(S): MARPAT 137:185360  
 GI



AB Halogenated calixpyrrole, calixpyridinopyrrole, and calixpyridine macrocycles, such as octabromo-meso-octamethylcalix[4]pyrrole (I) and calixpyridinopyrrole II, having 4-12 pyrrolic rings with greater stability were prepared for uses such as dialysis, ion exchange, and environmental remediation. Thus, I was prepared in 90% yield by bromination of the corresponding meso-octamethylcalix[4]pyrrole using N-bromosuccinimide in THF. Enhanced anion, neutral mol. binding affinity and different binding selectivities as compared to their nonhalogenated congeners as judged from <sup>1</sup>H NMR, <sup>19</sup>F NMR and fluorescence emission spectroscopic analyses.

IT **311804-81-6P**

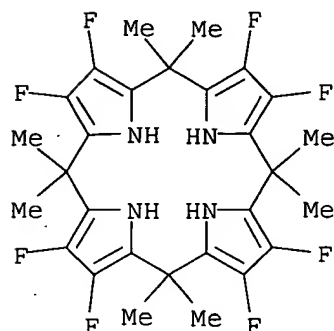
RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(preparation and anion binding properties of calixpyrroles, calixpyridinopyrroles and calixpyridines for use environmental remediation, kidney dialysis and cation exchangers)



RN 311804-81-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



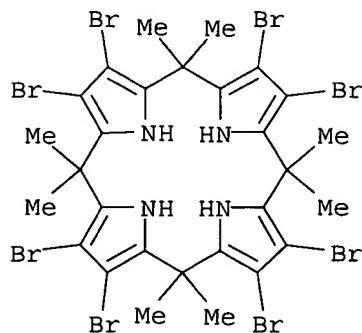
IT 190517-33-0P

RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(preparation and anion binding properties of calixpyrroles, calixpyridinopyrroles and calixpyridines for use environmental remediation, kidney dialysis and cation exchangers)

RN 190517-33-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



L13 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:593350 CAPLUS

DOCUMENT NUMBER: 138:73246

TITLE: Mono halogen substituted calix[4]pyrroles: fine-tuning the anion binding properties of calix[4]pyrrole

AUTHOR(S): Miyaji, Hidekazu; An, Deqiang; Sessler, Jonathan L.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, University of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Supramolecular Chemistry (2001), 13(6), 661-669

CODEN: SCHEER; ISSN: 1061-0278

PUBLISHER: Gordon & Breach Science Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Single halogen atom (i.e. I, Br, Cl and F) substituted calix[4]pyrroles, compds. were synthesized. Studies of these systems reveal that replacement of a single  $\beta$ -pyrrolic hydrogen atom can increase the



anion binding ability of calix[4]pyrroles for a variety of anions (e.g. Cl<sup>-</sup>, Br<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup> and HSO<sub>4</sub><sup>-</sup>) relative to normal non-halogen substituted calix[4]pyrrole. In the case of chloride anion, the expected relative affinity sequence of for these compds. was observed. This was not found to be true for Br<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, and HSO<sub>4</sub><sup>-</sup>. Here, the chlorine substituted calix[4]pyrrole was found to display a slightly higher affinity in the case of each anion than the fluorine-bearing derivative. This was rationalized in terms of intermol. NH...F hydrogen bonding interactions being present in CD<sub>2</sub>Cl<sub>2</sub> solns. of fluorine compound. Support for this latter conclusion came from concentration and temperature-dependent NMR spectroscopic studies.

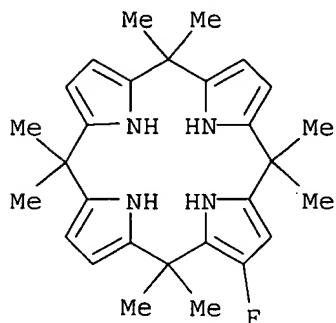
A matched set of mono halogen substituted calix[4]pyrroles was used to study in detail, the extent to which halogen substituents may be used to fine-tune the anion binding properties of calix[4]pyrroles.

IT 479669-58-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and anion binding properties and dimeric formation of monofluoro-substituted calix[4]pyrroles)

RN 479669-58-4 CAPLUS

CN 21H,23H-Porphine, 2-fluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)

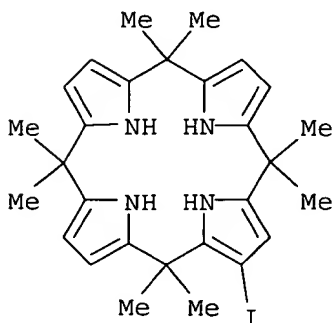


IT 265137-00-6P 479669-56-2P 479669-57-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and anion binding properties of monohalogen-substituted calix[4]pyrroles)

RN 265137-00-6 CAPLUS

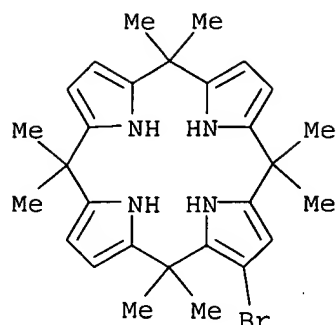
CN 21H,23H-Porphine, 5,10,15,20,22,24-hexahydro-2-iodo-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



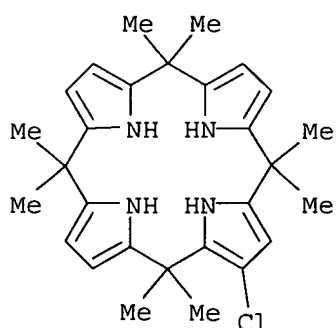
RN 479669-56-2 CAPLUS

CN 21H,23H-Porphine, 2-bromo-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)





RN 479669-57-3 CAPLUS  
 CN 21H,23H-Porphine, 2-chloro-5,10,15,20,22,24-hexahydro-  
 5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)

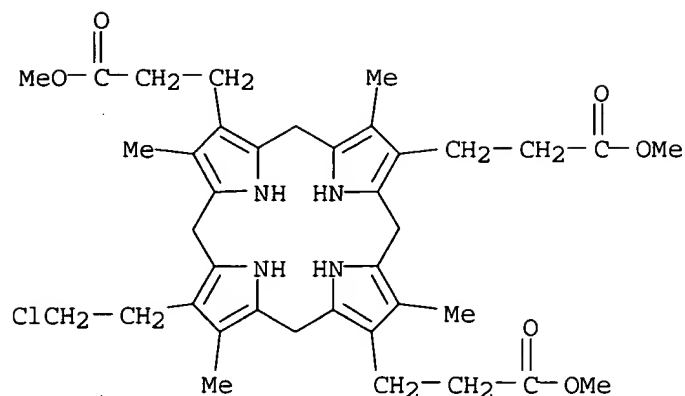


REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2002:211236 CAPLUS  
 DOCUMENT NUMBER: 137:43324  
 TITLE: Unprecedented overmetabolism of a porphyrinogen  
 substrate by coproporphyrinogen oxidase  
 AUTHOR(S): Lash, Timothy D.; Keck, Anna-Sigrid I. M.; Mani, Ukti  
 N.; Jones, Marjorie A.  
 CORPORATE SOURCE: Department of Chemistry, Illinois State University,  
 Normal, IL, 61790-4160, USA  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2002),  
 12(7), 1079-1082  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 137:43324  
 AB Harderoporphyrinogen-I is metabolized by avian hemolysate preps. of  
 coproporphyrinogen oxidase to give a trivinyl product; this  
 unprecedented 'overmetabolism' of the porphyrinogen substrate provides  
 strong support for a proposed model of the active site of this poorly  
 understood enzyme.  
 IT **438618-62-3P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (overmetabolism of porphyrinogen substrate provides support for active  
 site model of coproporphyrinogen oxidase)  
 RN 438618-62-3 CAPLUS  
 CN 21H,23H-Porphine-2,7,12-tripropionic acid, 17-(2-chloroethyl)-  
 5,10,15,20,22,24-hexahydro-3,8,13,18-tetramethyl-, trimethyl ester (9CI)



(CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:802778 CAPLUS

DOCUMENT NUMBER: 134:100852

TITLE: Direct Synthesis of Expanded Fluorinated Calix[n]pyrroles: Decafluorocalix[5]pyrrole and Hexadecafluorocalix[8]pyrrole

AUTHOR(S): Sessler, Jonathan L.; Anzenbacher, Pavel, Jr.; Shriver, James A.; Jursikova, Karolina; Lynch, Vincent M.; Marquez, Manuel

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, University of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Journal of the American Chemical Society (2000), 122(48), 12061-12062  
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:100852

AB Methanesulfonic acid-catalyzed condensation of 3,4-difluoropyrrole and acetone gives, in addition to octafluorocalix[4]pyrrole, the dominant reaction product, appreciable quantities of both the corresponding calix[5] and calix[8] products.

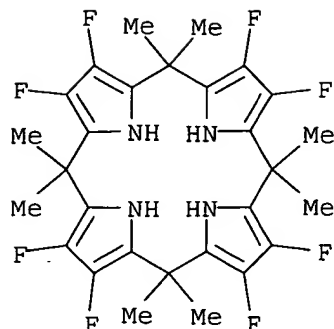
IT 311804-81-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of fluorinated calix[n]pyrroles)

RN 311804-81-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE.FORMAT

L13 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:713589 CAPLUS

DOCUMENT NUMBER: 134:29400

TITLE: Lithiation of meso-octamethylcalix[4]pyrrole: a general route to C-rim monosubstituted calix[4]pyrroles

AUTHOR(S): Anzenbacher, Pavel, Jr.; Jursikova, Karolina; Shriver, James A.; Miyaji, Hidekazu; Lynch, Vincent M.; Sessler, Jonathan L.; Gale, Philip A.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, University of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Journal of Organic Chemistry (2000), 65(22), 7641-7645  
CODEN: JOCEAH; ISSN: 0022-3263

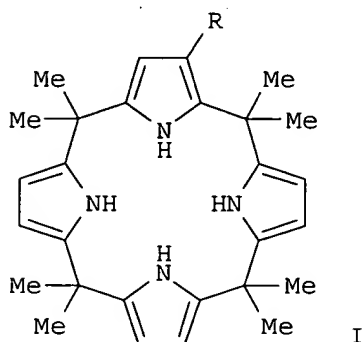
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:29400

GI



I

AB Lithiation and subsequent addition of an electrophile to meso-octamethylcalix[4]pyrrole provides a straightforward synthetic route to new, C-rim monosubstituted calix[4]pyrroles I (R = HO<sub>2</sub>C, EtO<sub>2</sub>CCH<sub>2</sub>, I, OHC, HOCH<sub>2</sub>CH<sub>2</sub>). A variety of electrophiles were used, resulting in calix[4]pyrroles with appended functional groups including carboxyl, ester, iodo, and formyl. This method was optimized to give maximum yields of the monosubstituted derivs. with lowest possible contamination by di- and trisubstituted congeners. Solid-state studies, performed for a number of these derivs., showed unexpected supramol. interactions involving both solvents and the monosubstituted calix[4]pyrrole derivs. themselves.

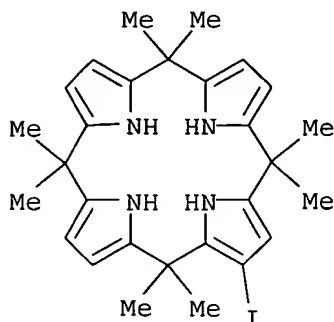


IT 265137-00-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of calixpyrrole derivs. via lithiation of  
octamethylcalixpyrrole followed by electrophilic addition)

RN 265137-00-6 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20,22,24-hexahydro-2-iodo-5,5,10,10,15,15,20,20-  
octamethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:707590 CAPLUS

DOCUMENT NUMBER: 134:29395

TITLE: Fluorinated Calix[4]pyrrole and Dipyrrolylquinoxaline:  
Neutral Anion Receptors with Augmented Affinities and  
Enhanced Selectivities

AUTHOR(S): Anzenbacher, Pavel, Jr.; Try, Andrew C.; Miyaji,  
Hidekazu; Jursikova, Karolina; Lynch, Vincent M.;  
Marquez, Manuel; Sessler, Jonathan L.

CORPORATE SOURCE: Department of Chemistry and Institute of  
for Cellular and Molecular Biology, University of  
Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Journal of the American Chemical Society (2000),  
122(42), 10268-10272

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Octamethyloctafluorocalix[4]pyrrole and 2,3-di(3,4-difluoropyrrol-2-  
yl)quinoxaline were prepared from 3,4-difluoro-1H-pyrrole. These latter two  
entities act as neutral anion receptors and bind anions such as fluoride,  
chloride, or dihydrogen phosphate with an enhanced affinity compared to  
their non-fluorinated congeners as judged from <sup>1</sup>H NMR, <sup>19</sup>F NMR, and  
fluorescence emission spectroscopic analyses. The increase in affinity  
was especially high in case of chloride and dihydrogen phosphate anion, with

the

2,3-di(3,4-difluoropyrrol-2-yl)quinoxaline system, in particular,  
displaying an affinity for H<sub>2</sub>PO<sub>4</sub><sup>-</sup> that was improved by 3 orders of  
magnitude as compared to its non-fluorinated congener. This improvement  
in the affinity for the dihydrogen phosphate is accompanied by change of  
color from pale yellow to orange, thus allowing the use of such compds. as  
naked-eye sensors for phosphate anion. In the case of the  
octafluorocalix[4]pyrrole system X-ray diffraction analyses revealed the  
presence of four different macrocyclic conformations in the solid state,  
as well as close intermol. contacts mediated by apparent CF<sup>-</sup> -HN hydrogen  
bonds.

IT 311804-81-6P

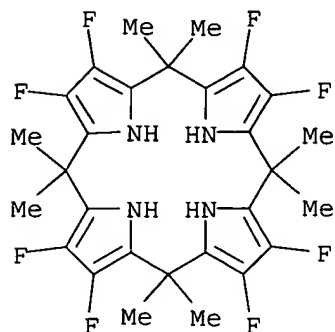
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)



(preparation and anion binding by octafluorooctamethylcalixpyrrole and bis(difluoropyrrolyl)quinoxaline)

RN 311804-81-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



IT 311804-87-2P 311804-88-3P 311804-89-4P  
311804-94-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and anion binding by octafluorooctamethylcalixpyrrole and bis(difluoropyrrolyl)quinoxaline)

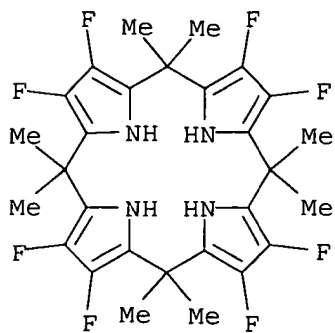
RN 311804-87-2 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, fluoride, compd. with  
2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-  
5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 311804-81-6

CMF C28 H28 F8 N4

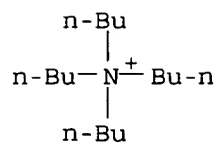


CM 2

CRN 429-41-4

CMF C16 H36 N . F





● F<sup>-</sup>

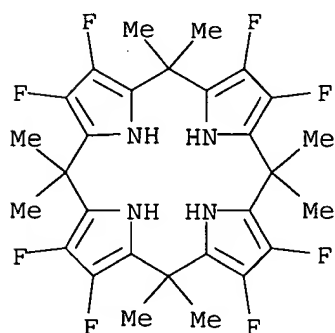
RN 311804-88-3 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, chloride, compd. with  
2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-  
5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX  
NAME)

CM 1

CRN 311804-81-6

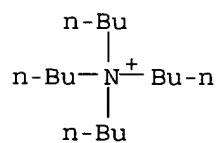
CMF C28 H28 F8 N4



CM 2

CRN 1112-67-0

CMF C16 H36 N . Cl



● Cl<sup>-</sup>

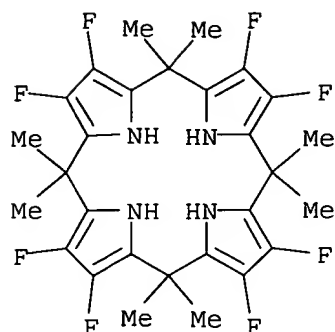
RN 311804-89-4 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, phosphate, compd. with  
2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-  
5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1:1) (9CI) (CA INDEX  
NAME)

CM 1



CRN 311804-81-6  
CMF C28 H28 F8 N4

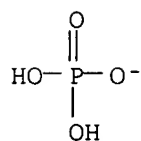


CM 2

CRN 5574-97-0  
CMF C16 H36 N . H2 O4 P

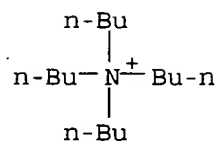
CM 3

CRN 14066-20-7  
CMF H2 O4 P



CM 4

CRN 10549-76-5  
CMF C16 H36 N

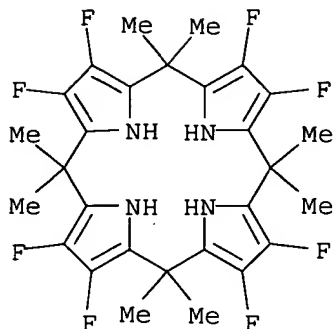


RN 311804-94-1 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-, compd. with sulfinylbis[methane] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 311804-81-6  
CMF C28 H28 F8 N4

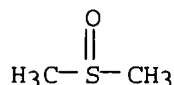




CM 2

CRN 67-68-5

CMF C2 H6 O S



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:595395 CAPLUS

DOCUMENT NUMBER: 133:335221

TITLE: Calix[4]pyrrole dimers bearing rigid spacers: towards the synthesis of cooperative anion binding agents

AUTHOR(S): Sato, W.; Miyaji, H.; Sessler, J. L.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, The University of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Tetrahedron Letters (2000), 41(35), 6731-6736

CODEN: TELEAY; ISSN: 0040-4039

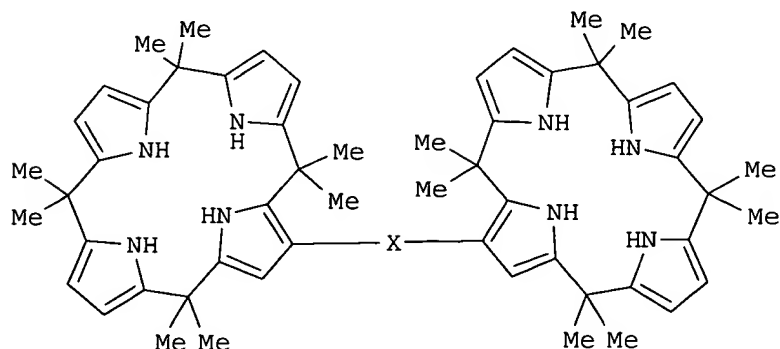
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:335221

GI



I

AB Calix[4]pyrrole dimers I [X = bond, p-C6H4, m-C6H4], potential hosts for



anionic guests, were synthesized by a procedure involving palladium(0) catalyzed C-C bond formation. In the case of I [X = bond] a detailed study of carboxylate anion binding was carried out using <sup>1</sup>H NMR spectroscopy. For isophthalate anion, a 1:1 binding stoichiometry was observed with this receptor and a much higher association constant was found

than

for the control monomer, octamethylcalix[4]pyrrole. These findings are ascribed to cooperative binding. Consistent with this conclusion was the finding that, for phthalate and benzoate anions, 1:2 (host:guest) binding stoichiometries and lower association consts. were recorded than with isophthalate anion. The control compound, octamethylcalix[4]pyrrole, showed a 1:1 binding stoichiometry and a much lower association constant than I [X = bond] not just with isophthalate but also phthalate and benzoate anions.

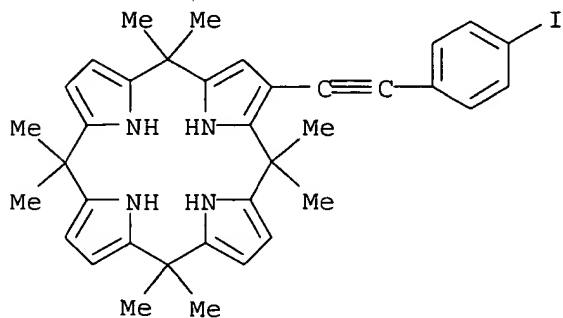
IT 303772-65-8P 303772-67-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and benzenecarboxylate binding of calix[4]pyrrole dimers with rigid spacers)

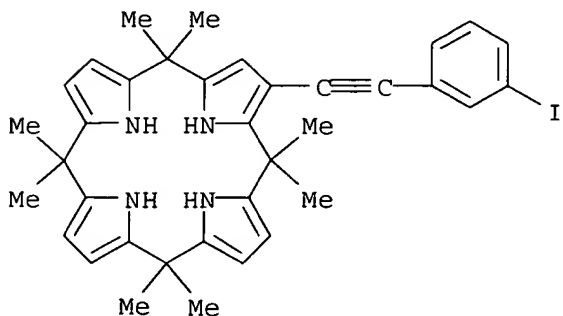
RN 303772-65-8 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20,22,24-hexahydro-2-[(4-iodophenyl)ethynyl]-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



RN 303772-67-0 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20,22,24-hexahydro-2-[(3-iodophenyl)ethynyl]-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:170492 CAPLUS

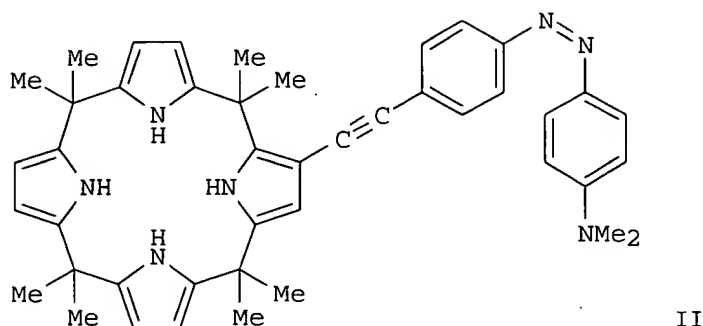
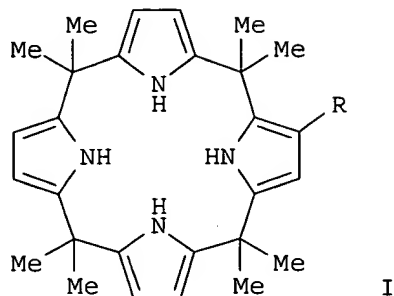
DOCUMENT NUMBER: 132:308324

TITLE: A "building block" approach to functionalized calix[4]pyrroles

AUTHOR(S): Miyaji, Hidekazu; Sato, Wataru; Sessler, Jonathan L.; Lynch, Vincent M.



CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute  
for Cellular and Molecular Biology, The University of  
Texas at Austin, Austin, TX, 78712-1167, USA  
SOURCE: Tetrahedron Letters (2000), 41(9), 1369-1373  
CODEN: TELEAY; ISSN: 0040-4039  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 132:308324  
GI



AB Iodocalix[4]pyrrole I (R = I) and trimethylsilyl ethynylcalix[4]pyrrole I (R = Me<sub>3</sub>SiC.tplbond.C) are key intermediates en route to the preparation of the alkynyl-substituted calix[4]pyrrole system I (R = HC.tplbond.C). I (R = HC.tplbond.C) in turn, provides a versatile precursor that can be used to prepare a range of arylalkynyl-functionalized calix[4]pyrroles such as II by the Sonogashira reaction of I (R = HC.tplbond.C) with appropriate aryl iodides R<sub>1</sub>I [R<sub>1</sub> = 4-MeC<sub>6</sub>H<sub>4</sub>, 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 2,4-(O<sub>2</sub>N)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 9-phenanthrenyl, 4-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>N:N-4-C<sub>6</sub>H<sub>4</sub>] in the presence of tetrakis(triphenylphosphine)palladium(0). Significant red-shifts in the λ<sub>max</sub> values and broadenings of the absorption peaks are seen in the UV-vis spectra of systems I [R = 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>C.tplbond.C, 2,4-(O<sub>2</sub>N)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>C.tplbond.C] upon addition of anions such as F<sup>-</sup>, Cl<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup> in CH<sub>2</sub>Cl<sub>2</sub>, a finding that leads to the suggestion that these or other analogous systems could find application as anion sensors.

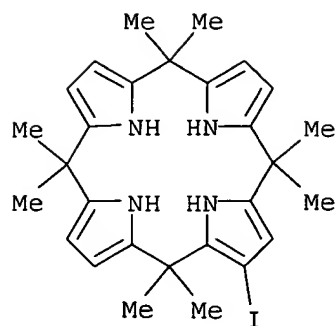
IT **265137-00-6P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of arylalkynyl calixpyrrole derivs. and their UV/visible spectra and anion binding properties)

RN 265137-00-6 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20,22,24-hexahydro-2-iodo-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:624263 CAPLUS

DOCUMENT NUMBER: 131:331398

TITLE: Oxidation of porphyrinogen

AUTHOR(S): He, Mingwei; Wang, Junwen; Wang, Yu; Ding, Jingfan; Zhou, Xiaoxi; Wen, Shufang

CORPORATE SOURCE: Dep. Chem., Shanxi Univ., Taiyuan, 030006, Peop. Rep. China

SOURCE: Huaxue Shiji (1999), 21(4), 201-204

CODEN: HUSHDR; ISSN: 0258-3283

PUBLISHER: Huagongbu Huaxue Shiji Xinsizhan

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB The effect of oxidizing agent such as nitrobenzene, inorg. oxidizing agent with standard electrode potential in the 0.25-0.36 V range on the synthesis of porphyrin was studied. K ferricyanide, arsenious acid and mercurous chloride can oxidize porphyrinogen to porphyrin. However, cupric and vanadyl acetylacetone can directly turn porphyrinogen into cupric porphyrin and vanadyl porphyrin. Yields of the title compds. are improved by choosing the right solvent. Also, b.p. and ET(30) of solvent are useful parameters in the selection of the solvent.

IT **248606-50-0P**

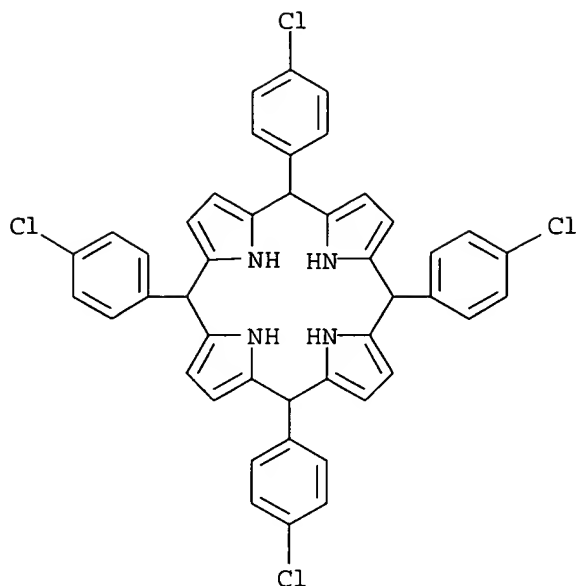
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, oxidation and reaction with copper and vanadyl acetylacetonato complexes)

RN 248606-50-0 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20-tetrakis(4-chlorophenyl)-5,10,15,20,22,24-hexahydro- (9CI) (CA INDEX NAME)





L13 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:684406 CAPLUS

DOCUMENT NUMBER: 127:346236

TITLE: preparation of calixpyrroles, calixpyridinopyrroles and calixpyridines

INVENTOR(S): Gale, Philip A.; Sessler, Jonathan L.; Genge, John W.; Kral, Vladimir; Andrievsky, Andrei; Lynch, Vincent; Sansom, Petra I.; Allen, William E.; et al.

PATENT ASSIGNEE(S): Board of Regents, the University of Texas System, USA

SOURCE: PCT Int. Appl., 145 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

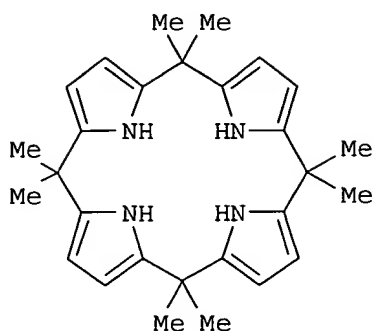
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9737995	A1	19971016	WO 1997-US5643	19970404
W:			AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM	
RW:			GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG	
CA 2251072	AA	19971016	CA 1997-2251072	19970404
CA 2391030	AA	19971016	CA 1997-2391030	19970404
AU 9724409	A1	19971029	AU 1997-24409	19970404
EP 891364	A1	19990120	EP 1997-920143	19970404
R:			CH, DE, FR, GB, IT, LI, NL, SE	
JP 2000511880	T2	20000912	JP 1997-536364	19970404
PRIORITY APPLN. INFO.:			US 1996-14890P	P 19960405
			US 1996-24203P	P 19960827
			US 1996-26694P	P 19960925
			US 1996-33395P	P 19961217
			US 1996-33396P	P 19961217
			CA 1997-2251072	A3 19970404
			WO 1997-US5643	W 19970404

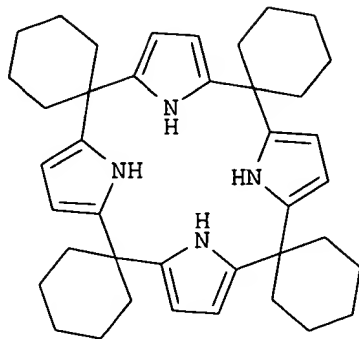


OTHER SOURCE(S) :  
GI

MARPAT 127:346236



I



II

AB Preparation of calixpyrrole, calixpyridinopyrrole, and calixpyridine macrocycles having 4, 5, 6, 7, or 8 heterocyclic rings, such as I and II, was described. Such macrocycles have proved to be effective and selective ion- and neutral mol.-binding agents forming supramol. ensembles, and ion- and neutral mol.-separation agents. The macrocycles are fully meso-non-hydrogen-substituted porphyrinogens, a few mols. of which were previously known but not recognized as possessing anion- or mol.-binding properties. The binding mode is noncovalent, primarily that of hydrogen-bonding, thereby providing a new mode for liquid chromatog., that of hydrogen bonding liquid chromatog. Further useful applications of the macrocycles include environmental remediation by removal of undesired ions or neutral mols., and removal of phosphate for kidney dialysis. Thus, calix[4]pyrrole I was prepared by cyclization of pyrrole and acetone in the presence of MeSO<sub>3</sub>H, which was added slowly to prevent a violent reaction. II was prepared by reaction of pyrrole with cyclohexanone in the presence of HCl. Stability consts. for I and II were determined to demonstrate their affinity for various ions in solution, e.g. giving a constant of  $350 \pm 5.5$  M<sup>-1</sup> for chloride.

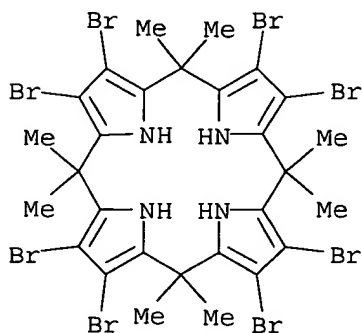
IT 190517-33-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of calixpyrroles, calixpyridinopyrroles and calixpyridines)

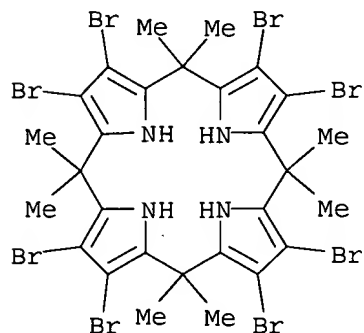
RN 190517-33-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)





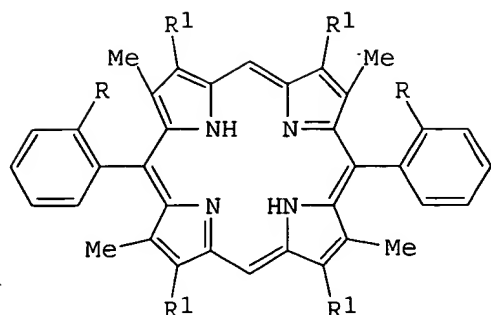
ACCESSION NUMBER: 1997:275704 CAPLUS  
 DOCUMENT NUMBER: 127:17652  
 TITLE: Calix[4]pyrroles: C-rim substitution and tunability of anion binding strength  
 AUTHOR(S): Gale, Philip A.; Sessler, Jonathan L.; Allen, William E.; Tvermoes, Nicolai A.; Lynch, Vincent  
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX, 78712-1167, USA  
 SOURCE: Chemical Communications (Cambridge) (1997), (7), 665-666  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Electron-rich and electron-deficient C-rim substituted calix[4]pyrroles are synthesized and the anion binding ability of these receptors is found to be dependent upon the C-rim substituents.  
 IT **190517-33-0P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and tunability of anion binding strength of calixpyrroles)  
 RN 190517-33-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1988:590098 CAPLUS  
 DOCUMENT NUMBER: 109:190098  
 TITLE: Studies on the conformation of 5,15-diarylporphyrins with (arylsulfonyl)oxy substituents  
 AUTHOR(S): Sanders, Georgine M.; Van Dijk, Marinus; Van Veldhuizen, Albertus; Van der Plas, Henk C.; Hofstra, Ulbert; Schaafsma, Tjeerd J.  
 CORPORATE SOURCE: Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.  
 SOURCE: Journal of Organic Chemistry (1988), 53(22), 5272-81  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 109:190098  
 GI





I

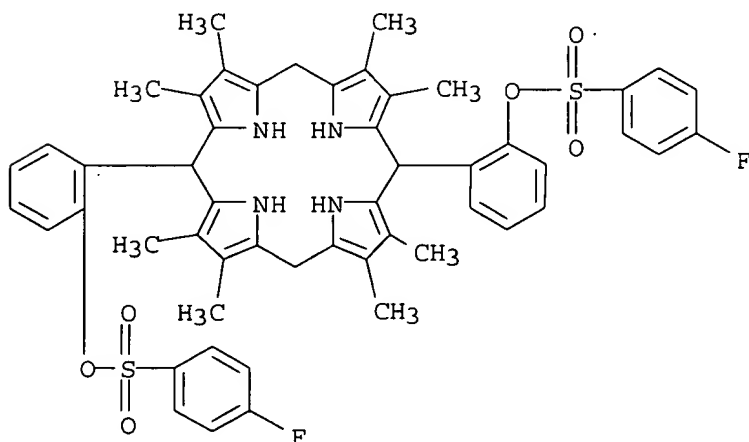
AB Octaalkylporphyrins, I (R = arylsulfonyloxyalkoxy, arylsulfonyloxy) and some related compds., were synthesized from dipyrrolylmethanes and aldehydes. On account of a  $^1\text{H}$ -NMR upfield shift in  $\text{CDCl}_3$  solution of 2-5 ppm for the aryl protons, a folded conformation is assumed in which the substituted aryl groups lie right above and below the porphyrin plane. In  $\text{CDCl}_3\text{-CF}_3\text{COOH}$  solution the upfield shifts are absent. The results of low-temperature  $^1\text{H}$ -NMR measurements and ring-current calcns. agreed with these assumptions. The sulfonyloxy group promotes folding of the mol. more than the ester, sulfonyl, sulfinyl, thio, or methylene group. In zinc porphyrins carrying anthraquinone substituents, intramol. coordination was observed.  $\Delta G$ ,  $\Delta H$ , and  $\Delta S$  values for the various conformational equilibrium were calculated from the NMR data. Van der Waals interactions with a contribution of charge transfer are suggested as the driving force for the folding of the mol.

IT 116748-14-2P 116748-23-3P 116748-25-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and dehydrogenation of)

RN 116748-14-2 CAPLUS

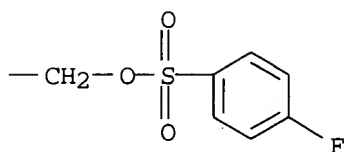
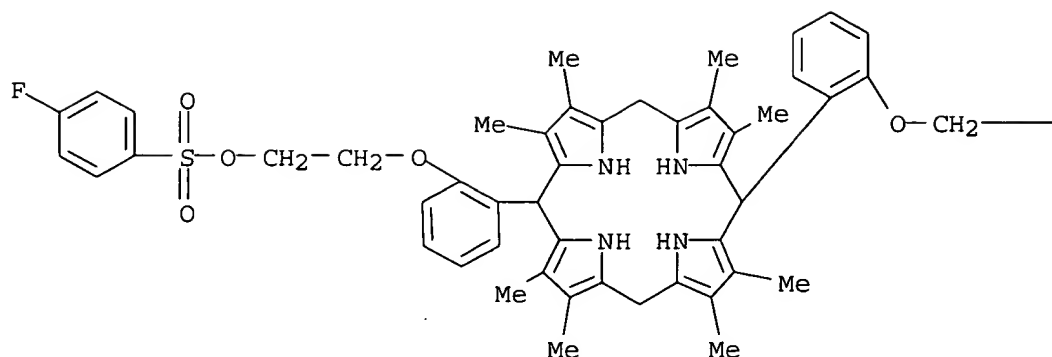
CN Benzenesulfonic acid, 4-fluoro-, (5,10,15,20,22,24-hexahydro-2,3,7,8,12,13,17,18-octamethyl-21H,23H-porphine-5,15-diyl)di-2,1-phenylene ester (9CI) (CA INDEX NAME)



RN 116748-23-3 CAPLUS

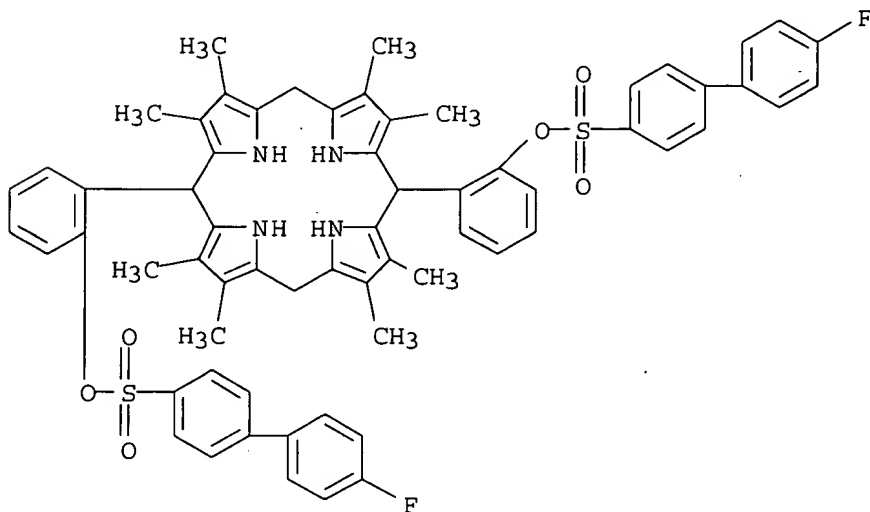
CN Benzenesulfonic acid, 4-fluoro-, (5,10,15,20,22,24-hexahydro-2,3,7,8,12,13,17,18-octamethyl-21H,23H-porphine-5,15-diyl)bis(2,1-phenyleneoxy-2,1-ethanediyl) ester (9CI) (CA INDEX NAME)





RN 116748-25-5 CAPLUS

CN [1,1'-Biphenyl]-4-sulfonic acid, 4'-fluoro-, (5,10,15,20,22,24-hexahydro-2,3,7,8,12,13,17,18-octamethyl-21H,23H-porphine-5,15-diyl) di-2,1-phenylene ester (9CI) (CA INDEX NAME)



L13 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1974:70790 CAPLUS

DOCUMENT NUMBER: 80:70790

TITLE: Synthetic studies on porphyrin systems

AUTHOR(S): Kenner, G. W.; Smith, K. M.

CORPORATE SOURCE: Robert Robinson Lab., Univ. Liverpool, Liverpool, UK

SOURCE: Annals of the New York Academy of Sciences (1973),  
206, 138-50



DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI For diagram(s), see printed CA Issue.

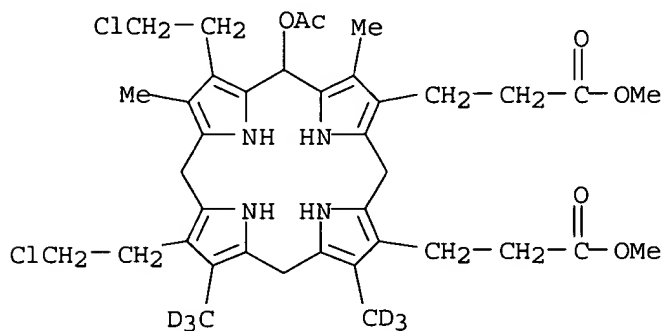
AB Specifically deuterated protoporphyrin-IX derivs., e.g. I, were prepared by several methods.

IT 51644-07-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 51644-07-6 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanoic acid, 5-(acetyloxy)-7,12-bis(2-chloroethyl)-5,10,15,20,22,24-hexahydro-3,8-dimethyl-13,17-di(methyl-d3)-, dimethyl ester (9CI) (CA INDEX NAME)



=&gt; s calixpyrrole

104 CALIXPYRROLE

35 CALIXPYRROLES

L14 116 CALIXPYRROLE

(CALIXPYRROLE OR CALIXPYRROLES)

=&gt; s l14 and anion binding

200185 ANION

107720 ANIONS

265434 ANION

(ANION OR ANIONS)

856548 BINDING

1886 BINDINGS

857077 BINDING

(BINDING OR BINDINGS)

1743 ANION BINDING

(ANION(W)BINDING)

L15 37 L14 AND ANION BINDING

=&gt; s l15 and tetrabutylammonium chloride

20957 TETRABUTYLAMMONIUM

1020760 CHLORIDE

151577 CHLORIDES

1089863 CHLORIDE

(CHLORIDE OR CHLORIDES)

1785 TETRABUTYLAMMONIUM CHLORIDE

(TETRABUTYLAMMONIUM(W)CHLORIDE)

L16 6 L15 AND TETRABUTYLAMMONIUM CHLORIDE

=&gt; d ibib abs hitstr l16 1-6

L16 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:495114 CAPLUS



DOCUMENT NUMBER: 140:111395  
TITLE: Synthesis and study of a **calixpyrrole**  
-texaphyrin chimera. A new oligopyrrolic chloride  
anion receptor  
AUTHOR(S): Sessler, Jonathan L.; Cho, Won-Seob; Dudek, Stephen  
P.; Hicks, Lindsay; Lynch, Vincent M.; Huggins,  
Michael T.  
CORPORATE SOURCE: Department of Chemistry & Biochemistry, The University  
of Texas at Austin, Austin, TX, 78712-0165, USA  
SOURCE: Journal of Porphyrins and Phthalocyanines (2003),  
7(2), 97-104  
CODEN: JPPHFZ; ISSN: 1088-4246  
PUBLISHER: Society of Porphyrins & Phthalocyanines  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Reported here is the synthesis and characterization of a new class of  
macrocycle that represents a hybrid between texaphyrin and  
**calixpyrrole**. These polypyrrolic macrocycles were prepared in one  
step by the acid-catalyzed condensation between diformyl dipyrromethanes  
and o-phenylenediamines in high yields. The X-ray crystal structure of  
one of these new "chimeras" was solved. It reveals that the diprotonated  
Schiff-base macrocycle has a V-shape in which one chloride anion is bound.  
Isothermal titration calorimetry (ITC) studies served to confirm the ability  
of the hybrid macrocycles to bind chloride anion in acetonitrile solution  
These compds. may be useful as easy-to-make anion receptors.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:385522 CAPLUS  
DOCUMENT NUMBER: 139:100832  
TITLE: Single Side Strapping: A New Approach to Fine Tuning  
the Anion Recognition Properties of Calix[4]pyrroles  
AUTHOR(S): Lee, Chang-Hee; Na, Hee-Kyung; Yoon, Dae-Wi; Won,  
Dong-Hoon; Cho, Won-Seob; Lynch, Vincent M.; Shevchuk,  
Sergey V.; Sessler, Jonathan L.  
CORPORATE SOURCE: Department of Chemistry, Kangwon National University,  
Chun-Chon, 200-701, S. Korea  
SOURCE: Journal of the American Chemical Society (2003),  
125(24), 7301-7306  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 139:100832

AB Three calix[4]pyrroles bearing m-ortcinol-derived diether straps of  
different lengths on one side of the tetrapyrrolic core were synthesized  
and characterized. Structural information for an analogous diester  
bridged strapped system reported previously (Yoon, D. W.; Hwang, H.; Lee,  
C. H. Angew. Chemical, Int. Ed. Engl. 2002, 41, 1757-1759) is also provided  
as are bromide and chloride anion affinities for all four systems determined by  
Isothermal Titration Calorimetry (ITC) in acetonitrile. Although both sets  
of the strapped calix[4]pyrroles displayed enhanced affinities for  
chloride and bromide anion, differences were seen among the various  
receptors that support the conclusion that the **anion**  
**binding** ability of **calixpyrrole**-type systems can be  
effectively tuned by modifying the length and nature of the bridging  
straps. In the specific case of the diether systems, the largest chloride  
affinity was seen with the shortest strap, whereas the largest affinity  
for bromide anion was recorded in the case of the longest strap. As well  
as supporting 1H NMR spectroscopic studies, it is postulated that not only  
cavity size per se, but also the ability of the aryl portion of the strap  
to serve as a CH H bond donor site are important in regulating the observed  
anion affinities.



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:593350 CAPLUS

DOCUMENT NUMBER: 138:73246

TITLE: Mono halogen substituted calix[4]pyrroles: fine-tuning the **anion binding** properties of calix[4]pyrrole

AUTHOR(S): Miyaji, Hidekazu; An, Deqiang; Sessler, Jonathan L.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, University of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Supramolecular Chemistry (2001), 13(6), 661-669  
CODEN: SCHEER; ISSN: 1061-0278

PUBLISHER: Gordon & Breach Science Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Single halogen atom (i.e. I, Br, Cl and F) substituted calix[4]pyrroles, compds. were synthesized. Studies of these systems reveal that replacement of a single  $\beta$ -pyrrolic hydrogen atom can increase the **anion binding** ability of calix[4]pyrroles for a variety of anions (e.g. Cl<sup>-</sup>, Br<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup> and HSO<sub>4</sub><sup>-</sup>) relative to normal non-halogen substituted calix[4]pyrrole. In the case of chloride anion, the expected relative affinity sequence of for these compds. was observed. This was not found to be true for Br<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, and HSO<sub>4</sub><sup>-</sup>. Here, the chlorine substituted calix[4]pyrrole was found to display a slightly higher affinity in the case of each anion than the fluorine-bearing derivative. This was rationalized in terms of intermol. NH...F hydrogen bonding interactions being present in CD<sub>2</sub>Cl<sub>2</sub> solns. of fluorine compound. Support for this latter conclusion came from concentration and temperature-dependent

NMR spectroscopic studies. A matched set of mono halogen substituted calix[4]pyrroles was used to study in detail, the extent to which halogen substituents may be used to fine-tune the **anion binding** properties of calix[4]pyrroles.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:653362 CAPLUS

DOCUMENT NUMBER: 135:357909

TITLE: First cryptand-like **calixpyrrole**: synthesis, x-ray structure, and **anion binding** properties of a bicyclic[3.3.3]nonapyrrole

AUTHOR(S): Bucher, Christophe; Zimmerman, Rebecca S.; Lynch, Vincent; Sessler, Jonathan L.

CORPORATE SOURCE: Department of Chemistry and Institute for Cellular and Molecular Biology, University of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Journal of the American Chemical Society (2001), 123(39), 9716-9717  
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

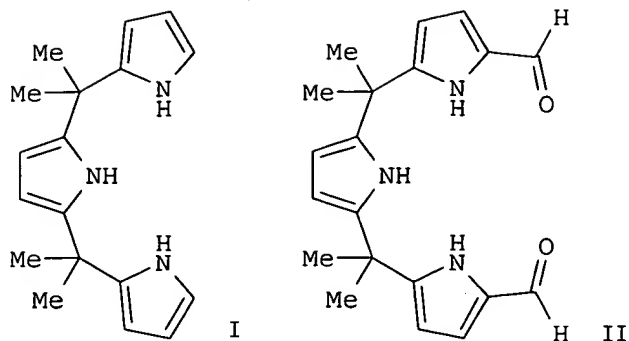
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:357909

GI





AB Bicyclic[3.3.3]nonapyrrole, a cryptand-like **calixpyrrole**, was prepared by reacting tripyrrane I with the tripyrrane dialdehyde II. The resulting bicyclic[3.3.3]nonapyrrole was examined by x-ray anal., which revealed that the mol. adopts an in-in configuration wherein both meso-like bridging carbon atoms are pointing in toward the center of the mol. The **anion binding** behavior of this compound was examined using a variety of tetrabutylammonium salts. Depending on the anion, the bicyclic[3.3.3]nonapyrrole was found to bind either via a slow or a fast equilibrium-binding process.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:570756 CAPLUS

DOCUMENT NUMBER: 133:321732

TITLE: Modified Calix[4]pyrroles

AUTHOR(S): Sessler, Jonathan L.; Anzenbacher, Pavel, Jr.; Miyaji, Hidekazu; Jursikova, Karolina; Bleasdale, Ellen R.; Gale, Philip A.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, University of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Industrial & Engineering Chemistry Research (2000), 39(10), 3471-3478

CODEN: IECRED; ISSN: 0888-5885

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:321732

AB The synthesis and chemical properties of a variety of chemical modified calix[4]pyrroles were described. The effects of structural changes, specifically the presence and absence of substituents on the meso-like and  $\beta$ -pyrrolic carbons, on anion affinities were detailed as was their effect on macrocycle conformation. Also described were unsym. systems, bearing an aliphatic and aromatic substituent on each of the four meso-like carbon atoms. In this case, the properties of the resulting configuration isomers are discussed in terms, again, of the resulting effects on macrocycle conformation and substrate binding affinity. Finally, the use of appropriately functionalized calix[4]pyrrole systems as rudimentary fluorescence-based anion sensors is presented.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:288186 CAPLUS

DOCUMENT NUMBER: 125:33102

TITLE: Calix[4]pyrroles: Old Yet New **Anion-Binding Agents**



AUTHOR(S): Gale, Philip A.; Sessler, Jonathan L.; Kral, Vladimir; Lynch, Vincent  
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Texas, Austin, TX, 78712-1167, USA  
 SOURCE: Journal of the American Chemical Society (1996), 118(21), 5140-5141  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The octaalkylporphyrinogens, octamethylcalix[4]pyrrole [i.e., 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine,] (I) and tetraspirocyclohexylcalix[4]pyrrole (II), have been found to be effective **anion binding** agents both in solution and in the solid state. Evidence for **anion binding** in the solid state derives from single crystal x-ray diffraction analyses with structures of the chloride complex of I and the fluoride complex of II being explicitly obtained. In these structures, the calix[4]pyrrole ligands are found in cone-like conformations such that the pyrrole NH protons can coordinate to the bound halide anions via hydrogen bonds. By contrast, x-ray structural analyses of the free receptors show that, in the absence of anions, compds. I and II adopt 1,3-alternate conformations in the solid state. Proton NMR titration studies, carried out in dichloromethane-d<sub>2</sub> solution, reveal that both compound are selective for fluoride over a variety of other anions (viz, Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup> and HSO<sub>4</sub><sup>-</sup>).

=> s 115 not 116  
 L17 31 L15 NOT L16

=> d ibib abs hitstr 117 1-31

L17 ANSWER 1 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2005:42063 CAPLUS  
 TITLE: Calix[4]bipyrrole-a big, flexible, yet effective chloride-selective anion receptor  
 AUTHOR(S): Sessler, Jonathan L.; An, Deqiang; Cho, Won-Seob; Lynch, Vincent; Marquez, Manuel  
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, Institute for Cellular and Molecular Biology, The University of Texas at Austin, Austin, TX, 78712-0165, USA  
 SOURCE: Chemical Communications (Cambridge, United Kingdom) (2005), (4), 540-542  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB **Anion binding** studies reveal that, in spite of its big size and flexible structure, calix[4]bipyrrole shows strong **anion binding** in general and good selectivity towards chloride anion in acetonitrile.

IT INDEXING IN PROGRESS

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:1048871 CAPLUS  
 DOCUMENT NUMBER: 142:155500  
 TITLE: **Anion-Binding Behavior of Hybrid Calixpyrroles**  
 AUTHOR(S): Sessler, Jonathan L.; An, Deqiang; Cho, Won-Seob; Lynch, Vincent; Yoon, Dae-Wi; Hong, Seong-Jin; Lee, Chang-Hee



CORPORATE SOURCE: Department of Chemistry and Biochemistry, Institute of Cellular and Molecular Biology, The University of Texas at Austin, Austin, TX, 78712-1167, USA  
SOURCE: Journal of Organic Chemistry (2005), 70(5), 1511-1517  
CODEN: JOCEAH; ISSN: 0022-3263  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Hybrid **calixpyrrole** systems are **calixpyrrole**-like macrocycles that are based on more than one type of small mol. building block. Structurally, these "mixed-breed" macrocycles differ from **calixpyrroles** in that some pyrrolic units in the latter are replaced by other heterocyclic units such as furan, thiophene, bipyrrole, and bithiophene. Although several such systems have been reported in recent years, only a few have been studied as possible anion receptors. In this paper, the results of detailed **anion binding** studies involving several prototypic systems are reported. Taken in concert, these results highlight the fact that some hybrid systems display anion affinities that are considerably weaker than those of the parent **calixpyrrole**. On the other hand, they also show that some are good receptors for "Y-shaped" anions, such as carboxylates, and that they bind these species with high affinity. These findings are strongly supported by solid-state structural studies, which reveal an interesting "cross binding mode" for the binding of carboxylate anions by the bis-thiophene, bis-pyrrole system.

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:978726 CAPLUS  
DOCUMENT NUMBER: 142:134571  
TITLE: Calix[4]pyrrole[2]carbazole: A New Kind of Expanded **Calixpyrrole**  
AUTHOR(S): Piatek, Piotr; Lynch, Vincent M.; Sessler, Jonathan L.  
CORPORATE SOURCE: Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX, 78712-0165, USA  
SOURCE: Journal of the American Chemical Society (2004), 126(49), 16073-16076  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The synthesis and **anion binding** properties of a new class of **calixpyrrole** analog, containing two carbazole subunits in lieu of two of the four acetone bridging elements normally found in calix[4]pyrrole, is described. The compound exists in a winglike structure in the solid state, as judged from single-crystal X-ray diffraction analyses of both the free system and its benzoate anion complex. Evidence for **anion binding** in dichloromethane solution was obtained from static fluorescent quenching expts.; these latter revealed a slight preference for acetate relative to other carboxylate anions (e.g., benzoate, oxalate, succinate), as well as various other anionic substrates (i.e., chloride and dihydrogen phosphate). No evidence of binding was observed in the case of bromide, nitrate, and hydrogen sulfate.

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:925092 CAPLUS  
DOCUMENT NUMBER: 141:349685  
TITLE: Density functional theory studies of  $\beta$ -substituent effect on conformational preference and **anion binding** ability of



calix[4]pyrroles  
AUTHOR(S): Wang, Di-Fei; Wu, Yundong  
CORPORATE SOURCE: Department of Chemistry, The Hong Kong University of  
Science & Technology, Hong Kong, Peop. Rep. China  
SOURCE: ARKIVOC (Gainesville, FL, United States) (2004), (9),  
96-110  
CODEN: AGFUAR  
URL: [http://www.arkat-usa.org/ark/journal/2004/I09\\_Yuan/CY-1155L/CY-1155L.pdf](http://www.arkat-usa.org/ark/journal/2004/I09_Yuan/CY-1155L/CY-1155L.pdf)  
PUBLISHER: Arkat USA Inc.  
DOCUMENT TYPE: Journal; (online computer file)  
LANGUAGE: English

AB The conformational features and **anion-binding** properties of a series of  $\beta$ -octasubstituted calix[4]pyrroles have been investigated by the BLYP method of d. functional theory with the 6-31+G\*\* basis set both in the gas phase and in CH<sub>2</sub>Cl<sub>2</sub> solution. The calcns. demonstrated that adjusting the electronic properties of  $\beta$ -substituents on the pyrrole rings do change the **anion-binding** ability of calix[4]pyrroles. With the BLYP/6-31+G\*\* method in CH<sub>2</sub>Cl<sub>2</sub> solution, the relative binding energies follow the order of electron withdrawing abilities of the substituents, i.e. CN (18 kcal/mol) >> Cl (7 kcal/mol) > Br (4 kcal/mol) > H (0 kcal/mol). Calcns. also indicate that the energy difference between the most stable 1,3-alternate conformation and the least stable cone-conformation that is for **anion-binding** is increased by electron-withdrawing  $\beta$ -substituents CN, Cl, and Br. Further anal. on dipyrromethane models reveals that the destabilization of the cone-conformation is mainly caused by electrostatic interactions between the  $\beta$ -substituents on the adjacent pyrrole rings. Our results thus provide useful information for designing stronger and more efficient calix[4]pyrrole-based **anion binding** receptors.

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

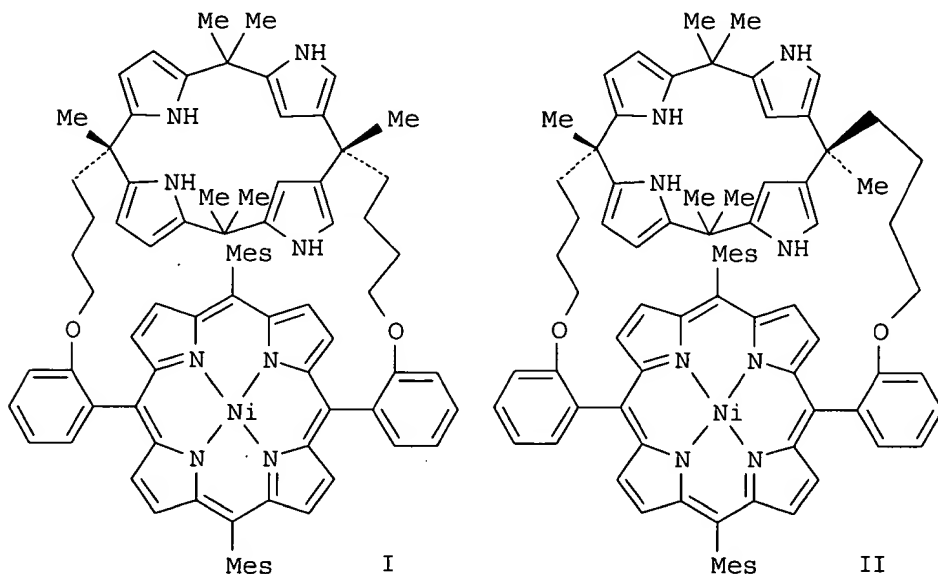
ACCESSION NUMBER: 2004:225081 CAPLUS  
TITLE: Oligopyrrole-based **anion binding** agents  
AUTHOR(S): Sessler, Jonathan L.; Gale, Philip A.; Anzenbacher, Pavel; Kral, Vladimir; Moyer, B. A.; Marquez, Manuel; Cho, Won-Seob; An, Deqiang; Shriver, James; Fowler, Christopher J.; Levitskaia, Tatiana G.; Magda, Darren J.  
CORPORATE SOURCE: Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX, 7812-0165, USA  
SOURCE: Abstracts of Papers, 227th ACS National Meeting, Anaheim, CA, United States, March 28-April 1, 2004 (2004), IEC-042. American Chemical Society: Washington, D. C.  
CODEN: 69FGKM  
DOCUMENT TYPE: Conference; Meeting Abstract  
LANGUAGE: English

AB Anion recognition is an important problem that is of critical relevance to a range of processes, both biol. and abiol. In this presentation, the use of protonated expanded porphyrins and neutral calix[n]pyrroles as receptors for anions will be reviewed. Synthetic methods leading to the preparation of calix[n]pyrroles, where  $n > 4$ , will be highlighted, as will be preparative work that leads to the preparation of so-called "expanded **calixpyrroles**", including those based on bipyrrolic precursors. Related work that provides open chain pyrrole-based receptors, including dipyrrolylquinoxalines and analogs as colorimetric sensors will be highlighted, as will be recent studies designed to highlight the potential biol. utility of these systems. Applications in anion extraction and separation



will also be prominently featured in this presentation.

L17 ANSWER 6 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2004:108677 CAPLUS  
DOCUMENT NUMBER: 140:331304  
TITLE: Calix[4]pyrrole-Capped Metalloporphyrins as Ditopic  
Receptor Models for Anions  
AUTHOR(S): Panda, Pradeepta K.; Lee, Chang-Hee  
CORPORATE SOURCE: Department of Chemistry, Kangwon National University,  
Chun-Chon, 200-701, S. Korea  
SOURCE: Organic Letters (2004), 6(5), 671-674  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Strapped calix[4]pyrrole-metalloporphyrin conjugates, potential hosts for anionic guests, were synthesized and characterized. The condensation unexpectedly gave the two cis-trans isomers of calix[4]pyrrole-capped porphyrins I and II. The **anion binding** studies revealed that only isomer I showed strong binding with fluoride anion in organic solvent, and neither isomer showed any appreciable binding with Cl<sup>-</sup>, Br<sup>-</sup>, and I<sup>-</sup>.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 7 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2003:635666 CAPLUS  
TITLE: Bipyrrole-based new **calixpyrrole** family members: Calix[n]bipyrroles, calix[2]bipyrrole[2]thiophene, and calix[2]bipyrrole[2]furan  
AUTHOR(S): Sessler, Jonathan L.; An, Deqiang; Cho, Won-Seob; Lynch, Vincent  
CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute of Cellular and Molecular Biology, The University of Texas at Austin, Austin, TX, 78712, USA



SOURCE: Abstracts of Papers, 226th ACS National Meeting, New York, NY, United States, September 7-11, 2003 (2003), ORGN-580. American Chemical Society: Washington, D. C.  
CODEN: 69EKY9

DOCUMENT TYPE: Conference; Meeting Abstract  
LANGUAGE: English

AB Rather than pyrrole, bipyrrrole has been incorporated as a key heterocyclic subunit in the design and synthesis of new members of the generalized **calixpyrrole** family. One set of these new macrocycles consists of calix[n]bipyrrroles (2, 3), and the other hybrids of bipyrrrole with thiophene (4) and furan (5). **Anion binding** studies reveal that receptor (2) binds large halide anions with affinities that are substantially enhanced relative to those of calix[4]pyrrole (1). Studies of these new receptors will help us understand how adjustments in receptor size, shape and hydrogen bond donor number affect the **anion binding** selectivities and affinities. Details of the synthesis and **anion binding** studies of these new receptors are presented in this poster.

L17 ANSWER 8 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2003:623230 CAPLUS  
DOCUMENT NUMBER: 139:370552  
TITLE: Fluorinated **calixpyrroles: anion-binding** extractants that reduce the Hofmeister bias  
AUTHOR(S): Levitskaia, Tatiana G.; Marquez, Manuel; Sessler, Jonathan L.; Shriver, James A.; Vercouter, Thomas; Moyer, Bruce A.  
CORPORATE SOURCE: Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37830-6119, USA  
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (17), 2248-2249  
CODEN: CHCOFS; ISSN: 1359-7345  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB  $\beta$ -Octafluoro-meso-octamethylcalix[4]pyrrole (I) and  $\beta$ -decafluoro-meso-decamethylcalix[5]pyrrole (II) were found to extract cesium salts of smaller anions (bromide and chloride for I and nitrate for II) as effectively as that of iodide into nitrobenzene (NB) thereby overcoming the Hofmeister bias normally observed for processes of this type.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 9 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2003:406063 CAPLUS  
DOCUMENT NUMBER: 140:93797  
TITLE: Pyrrolic and polypyrrolic **anion binding** agents  
AUTHOR(S): Sessler, Jonathan L.; Camiolo, Salvatore; Gale, Philip A.  
CORPORATE SOURCE: Institute for Cellular and Molecular Biology, Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX, 78712-0165, USA  
SOURCE: Coordination Chemistry Reviews (2003), 240(1-2), 17-55  
CODEN: CCHRAM; ISSN: 0010-8545  
PUBLISHER: Elsevier Science B.V.  
DOCUMENT TYPE: Journal; General Review  
LANGUAGE: English

AB A review which traces the emergence of pyrrole-based receptors for anion recognition. It outlines how serendipitous findings that the diprotonated form of sapphyrin, a pentapyrrolic expanded porphyrin, formed a



centrally-bound complex with fluoride anion made over a decade ago spawned studies of this and other expanded porphyrins as receptors, carriers, and sensors of anions. Further evolutions of the field, including in particular the finding that neutral, non-aromatic oligopyrrole macrocycles, such as the **calixpyrroles** and calixphyrins, can act as cheap, and easy-to-prepare anion receptors will also be highlighted, as will recent work with acyclic systems, including dipyrrolylquinoxalines (DPQs) and simple derivs. of pyrrole itself.

REFERENCE COUNT: 102 THERE ARE 102 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 10 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:751572 CAPLUS

DOCUMENT NUMBER: 137:389723

TITLE: Theoretical Study of **Anion Binding** to Calix[4]pyrrole: the Effects of Solvent, Fluorine Substitution, Cosolute, and Water Traces

AUTHOR(S): Blas, J. Ramon; Marquez, Manuel; Sessler, Jonathan L.; Luque, F. Javier; Orozco, Modesto

CORPORATE SOURCE: Departament de Bioquímica i Biologia Molecular, Facultat de Química, Universitat de Barcelona, Barcelona, 08028, Spain

SOURCE: Journal of the American Chemical Society (2002), 124(43), 12796-12805  
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The binding of different anions to calix[4]pyrrole has been studied by means of mol. dynamics coupled to thermodyn. integration calcns. The effect of different apolar solvents, octafluoro substitution, and the change in binding free energy derived from the presence of cosolute and water traces (the hydrated salt used to introduce the anion in the solution) were examined. Calcns. allow us to rationalize the differential binding of ions to calix[4]pyrrole and octafluorocalix[4]pyrrole as well as to predict the behavior in new solvents for which exptl. data are not available yet. It is found that both calix[4]pyrrole and octafluorocalix[4]pyrrole have a dramatic preference for F<sup>-</sup> in the gas phase and pure aprotic solvents, but the situation can change dramatically in protic solvents or in the presence of the hydrated cation which is used as cosolute of the anion. Overall, our results provide interesting clues for a better understanding of the process detected exptl. as "binding".

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 11 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:638268 CAPLUS

DOCUMENT NUMBER: 137:185360

TITLE: Preparation, binding properties, and uses of halogenated **calixpyrroles**, calixpyridinopyrroles and calixpyridines

INVENTOR(S): Sessler, Jonathan L.; Marquez, Manuel; Anzenbacher, Pavel; Shriver, James A.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 104 pp., Cont.-in-part of U.S. Ser. No. 838,998.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.

KIND

DATE

APPLICATION NO.

DATE



US 2002115566	A1	20020822	US 2001-939514	20010824
CA 2391030	AA	19971016	CA 1997-2391030	19970404
US 6262257	B1	20010717	US 1997-833379	19970404
US 2002026047	A1	20020228	US 2001-838998	20010420
WO 2003018548	A2	20030306	WO 2002-US27252	20020826
WO 2003018548	A3	20030703		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

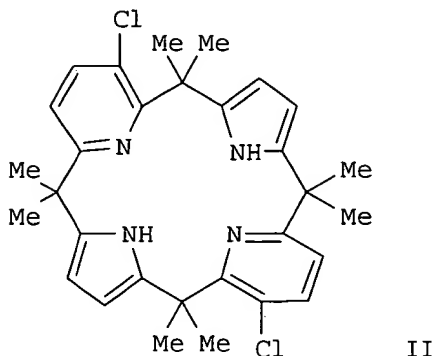
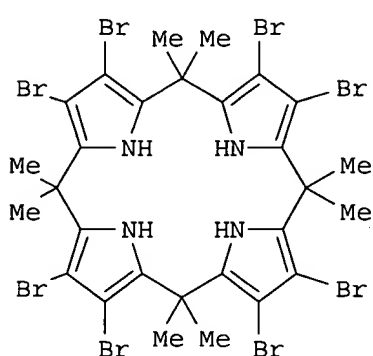
PRIORITY APPLN. INFO.:

US 1996-14890P	P	19960405
US 1996-24203P	P	19960827
US 1996-26694P	P	19960925
US 1996-33395P	P	19961217
US 1996-33396P	P	19961217
US 1997-833379	A3	19970404
US 2001-838998	A2	20010420
CA 1997-2251072	A3	19970404
US 2001-939514	A	20010824

OTHER SOURCE(S):

MARPAT 137:185360

GI



AB Halogenated **calixpyrrole**, calixpyridinopyrrole, and calixpyridine macrocycles, such as octabromo-meso-octamethylcalix[4]pyrrole (I) and calixpyridinopyrrole II, having 4-12 pyrrolic rings with greater stability were prepared for uses such as dialysis, ion exchange, and environmental remediation. Thus, I was prepared in 90% yield by bromination of the corresponding meso-octamethylcalix[4]pyrrole using N-bromosuccinimide in THF. Enhanced anion, neutral mol. binding affinity and different binding selectivities as compared to their nonhalogenated congeners as judged from <sup>1</sup>H NMR, <sup>19</sup>F NMR and fluorescence emission spectroscopic analyses.

L17 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:531760 CAPLUS

DOCUMENT NUMBER: 137:232636

TITLE: The Elusive  $\beta$ -Unsubstituted Calix[5]pyrrole  
Finally Captured

AUTHOR(S): Cafeo, Grazia; Kohnke, Franz H.; Parisi, Melchiorre  
F.; Nascone, Rosetta Pistone; La Torre, Giovanna L.;  
Williams, David J.



CORPORATE SOURCE: Dipartimento di Chimica Organica e Biologica,  
Universita di Messina, Messina, I-98166, Italy  
SOURCE: Organic Letters (2002), 4(16), 2695-2697  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 137:232636  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Decamethyl calix[5]pyrrole I was prepared from the calix[5]furan II by a three-step procedure; the crystal structure and **anion-binding** affinity of I were determined. Oxidative cleavage of the furan rings in II with mCPBA in CHCl<sub>3</sub> gave a cyclic pentaunsatd. pentadocosadecaone in 56% yield which was reduced with zinc in acetic acid to give a saturated cyclic decaketone in 97% yield; treatment of the cyclic decaketone with ammonium acetate in EtOH gave I in approx. 1% yield. In the crystal structure of I, the pyrrole rings of I tilt in alternating directions. I binds fluoride ion more tightly than the analogous calix[4]pyrrole but binds chloride ion less tightly than the analogous calix[4]pyrrole.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:418592 CAPLUS  
DOCUMENT NUMBER: 137:325289  
TITLE: Synthesis of a strapped calix[4]pyrrole: Structure and **anion binding** properties  
AUTHOR(S): Yoon, Dae-Wi; Hwang, Hoon; Lee, Chang-Hee  
CORPORATE SOURCE: Department of Chemistry, Kangwon National University, Chun-Chon, 200-701, S. Korea  
SOURCE: Angewandte Chemie, International Edition (2002), 41(10), 1757-1759  
CODEN: ACIEF5; ISSN: 1433-7851  
PUBLISHER: Wiley-VCH Verlag GmbH  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 137:325289

AB Enhanced affinity and selectivity for halide anions is seen for the strapped calix[4]pyrrole with F<sup>-</sup>, Cl<sup>-</sup> relative to normal calix[4]pyrroles. The encapsulated binding site differentiates the anions on the basis of size, and the existence of hydrogen-bonding interactions between the aromatic proton and halide anions has been verified by 1H NMR spectroscopy. A binding constant of approx. 3.87 × 10<sup>6</sup>M was found for the fluoride complex.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:35455 CAPLUS  
DOCUMENT NUMBER: 136:232037  
TITLE: Surprises in the Energetics of Host-Guest **Anion Binding** to Calix[4]pyrrole  
AUTHOR(S): Schmidtchen, Franz P.  
CORPORATE SOURCE: Institut fuer Organische Chemie und Biochemie, Technische Universitaet Muenchen, Garching, D-85747, Germany  
SOURCE: Organic Letters (2002), 4(3), 431-434



CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Contrary to common expectation, calorimetric measurements do not corroborate the preference of calix[4]pyrrole for fluoride over chloride in acetonitrile solution

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 15 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:812034 CAPLUS

DOCUMENT NUMBER: 136:85684

TITLE: Calixpyrins. Hybrid macrocycles at the structural crossroads between porphyrins and **calixpyrroles**

AUTHOR(S): Sessler, Jonathan L.; Zimmerman, Rebecca S.; Bucher, Christophe; Kral, Vladimir; Andrioletti, Bruno

CORPORATE SOURCE: Department of Chemistry & Biochemistry and the Institute for Cellular and Molecular Biology, The University of Texas, Austin, TX, 78712, USA

SOURCE: Pure and Applied Chemistry (2001), 73(7), 1041-1057  
CODEN: PACHAS; ISSN: 0033-4545

PUBLISHER: International Union of Pure and Applied Chemistry

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review. Calixpyrins are a class of hybrid mols. that lie at the structural crossroads between porphyrins and **calixpyrroles**. Porphyrins, long known for their versatile metal cation coordination chemical, are macrocycles that contain only sp<sup>2</sup>-hybridized bridging meso carbon atoms within their framework. Calix[n]pyrroles, on the other hand, are porphyrin analogs that contain pyrroles bridged exclusively by sp<sup>3</sup> meso carbon centers, and in recent years have been shown to display remarkable **anion-binding** properties. Calix[n]pyrins bear analogy to both the porphyrins and **calixpyrroles** and are macrocyclic analogs that contain a mixture of sp<sup>2</sup>- and sp<sup>3</sup>-hybridized meso carbon bridges. This leads to partial interruptions in the conjugation pathway of the mol., introduces novel structural features, and leads to interesting anion and cation recognition properties. It also allows for modular syntheses. In the present paper, the chemical of calix[n]pyrins, still at an early stage of exploration, is reviewed.

REFERENCE COUNT: 104 THERE ARE 104 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:639123 CAPLUS

TITLE: Polypyrrole-based **anion binding** agents

AUTHOR(S): Sessler, Jonathan L.; Kral, Vladimir; Gale, Philip A.; Anzenbacher, Pavel, Jr.; Davis, Julian A.; Bucher, Christophe; Shriver, James; Zimmerman, Rebecca; Miyaji, Hidekazu; Genge, John; Andrioletti, Bruno; Try, Andrew; Black, Christopher B.; Marquez, Manuel

CORPORATE SOURCE: Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX, 7812-1167, USA

SOURCE: Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, United States, August 26-30, 2001 (2001), IEC-069. American Chemical Society: Washington, D. C.  
CODEN: 69BUZP

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB In recent years pyrrole-based systems have emerged as important



**anion binding** motifs. In contrast to other substructures used to effect the recognition of anions, pyrroles appear especially attractive in that they remain neutral in most common organic solvents

and over a wide range of pH when exposed to aqueous media. In this Tutorial Lecture, the synthesis and **anion binding** properties of a number of polypyrrole anion recognition systems, both macrocyclic and acyclic, will be detailed and their possible use in applications ranging from waste remediation, anion sensing, oligonucleotide separation, and through-membrane transport will be reviewed. Particular emphasis will be placed on sapphyrins, **calixpyrroles**, dipyrrolylquinoxalines, and calix[n]pyrins. However, ongoing work involving 3-dimensional polypyrrolic cryptand systems will also be presented.

L17 ANSWER 17 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:298502 CAPLUS

DOCUMENT NUMBER: 135:107177

TITLE: Conformational Features and **Anion-Binding** Properties of Calix[4]pyrrole: A Theoretical Study

AUTHOR(S): Wu, Yun-Dong; Wang, Di-Fei; Sessler, Jonathan L.

CORPORATE SOURCE: Department of Chemistry, The Hong Kong University of Science and Technology, Kowloon Hong Kong, Peop. Rep. China

SOURCE: Journal of Organic Chemistry (2001), 66(11), 3739-3746  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The conformational preference of calix[4]pyrrole and its fluoride and chloride **anion-binding** properties have been investigated by d. functional theory calcns. Geometries were optimized by the BLYP/3-21G and BLYP/6-31G\* methods, and energies were evaluated with the BLYP/6-31+G\*\* method. To model the effect of medium, the SCIPCM solvent model was also employed. Four typical conformations of the parent substituent-free calix[4]pyrrole were studied. Both in the gas phase and in CH<sub>2</sub>Cl<sub>2</sub> solution, the stability sequence is predicted to be 1,3-alternate > partial cone > 1,2-alternate > cone. The cone conformation is predicted to be about 16.0 and 11.4 kcal/mol less stable in the gas phase and CH<sub>2</sub>Cl<sub>2</sub> solution, resp. This is mainly due to electrostatic repulsions arising from the all-syn pyrrole/pyrrole/pyrrole/pyrrole arrangement present in this conformer. The existence of possible 1:1 and 1:2 **anion-binding** modes were explored in the case of fluoride anion, and the factors favoring the 1:1 binding mode are discussed. The calculated binding energy for fluoride anion is about 15 kcal/mol larger than that for chloride anion. The calculated binding energy for chloride anion agrees with the exptl. value very well. The presence of meso-alkyl substituents destabilizes the cone conformer with respect to the 1,3-alternate conformer and, therefore, reduces the **anion-binding** affinity by 3-4 kcal/mol. The strength of N-H- -anion hydrogen bonds in the various structures subject to study were estimated on the basis of the calculated **anion-binding** energies and the predicted structural deformation energies of substituent-free calix[4]pyrrole.

REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 18 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:8057 CAPLUS

DOCUMENT NUMBER: 134:280479

TITLE: Selective **anion binding** and solid-state host-guest chemistry of an extended cavity calix[6]pyrrole

AUTHOR(S): Turner, Boaz; Shterenberg, Alexander; Kapon, Moshe; Eichen, Yoav; Suwinska, Kinga



CORPORATE SOURCE: Department of Chemistry, Technion-Israel Institute of  
Technology, Technion City, Haifa, 32000, Israel  
SOURCE: Chemical Communications (Cambridge) (2001), (1), 13-14  
CODEN: CHCOFS; ISSN: 1359-7345  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Easily prepared, cone-like, extended cavity calix[6]pyrrole is shown to form  
strong complexes with iodine and other halide ions as well as with  
trihaloalkanes and electron deficient aromatic systems.  
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 19 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:707590 CAPLUS  
DOCUMENT NUMBER: 134:29395  
TITLE: Fluorinated Calix[4]pyrrole and Dipyrrolylquinoxaline:  
Neutral Anion Receptors with Augmented Affinities and  
Enhanced Selectivities  
AUTHOR(S): Anzenbacher, Pavel, Jr.; Try, Andrew C.; Miyaji,  
Hidekazu; Jursikova, Karolina; Lynch, Vincent M.;  
Marquez, Manuel; Sessler, Jonathan L.  
CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute  
for Cellular and Molecular Biology, University of  
Texas at Austin, Austin, TX, 78712-1167, USA  
SOURCE: Journal of the American Chemical Society (2000),  
122(42), 10268-10272  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Octamethyloctafluorocalix[4]pyrrole and 2,3-di(3,4-difluoropyrrol-2-  
yl)quinoxaline were prepared from 3,4-difluoro-1H-pyrrole. These latter two  
entities act as neutral anion receptors and bind anions such as fluoride,  
chloride, or dihydrogen phosphate with an enhanced affinity compared to  
their non-fluorinated congeners as judged from <sup>1</sup>H NMR, <sup>19</sup>F NMR, and  
fluorescence emission spectroscopic analyses. The increase in affinity  
was especially high in case of chloride and dihydrogen phosphate anion, with  
the 2,3-di(3,4-difluoropyrrol-2-yl)quinoxaline system, in particular,  
displaying an affinity for H<sub>2</sub>PO<sub>4</sub><sup>-</sup> that was improved by 3 orders of  
magnitude as compared to its non-fluorinated congener. This improvement  
in the affinity for the dihydrogen phosphate is accompanied by change of  
color from pale yellow to orange, thus allowing the use of such compds. as  
naked-eye sensors for phosphate anion. In the case of the  
octafluorocalix[4]pyrrole system X-ray diffraction analyses revealed the  
presence of four different macrocyclic conformations in the solid state,  
as well as close intermol. contacts mediated by apparent CF- -HN hydrogen  
bonds.  
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:626125 CAPLUS  
DOCUMENT NUMBER: 133:328877  
TITLE: Second Generation **Calixpyrrole** Anion Sensors  
AUTHOR(S): Anzenbacher, Pavel, Jr.; Jursikova, Karolina; Sessler,  
Jonathan L.  
CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute  
for Cellular and Molecular Biology, University of  
Texas at Austin, Austin, TX, 78712-1167, USA  
SOURCE: Journal of the American Chemical Society (2000),  
122(38), 9350-9351  
CODEN: JACSAT; ISSN: 0002-7863



PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The authors report the synthesis of three 2nd generation **calixpyrrole**-based fluorescent anion sensors, compds. 1-3. These systems bind anions with greater affinity than previous systems while displaying a more efficient fluorescent response. In the design of sensors 1-3, a rigid aromatic spacer was used so as to fix the distance between the quencher (anion) and the signaling moiety. This spacer element contained either a sulfonamide (compound 1 and 2) or thiourea (sensor 3) group. These linker moieties were introduced with the expectation that they might provide addnl. H bond donor sites that would act in concert with the **calixpyrrole** NH protons to enhance the overall **anion binding** affinities.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 21 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:595395 CAPLUS

DOCUMENT NUMBER: 133:335221

TITLE: Calix[4]pyrrole dimers bearing rigid spacers: towards the synthesis of cooperative **anion binding** agents

AUTHOR(S): Sato, W.; Miyaji, H.; Sessler, J. L.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, The University of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Tetrahedron Letters (2000), 41(35), 6731-6736

CODEN: TELEAY; ISSN: 0040-4039

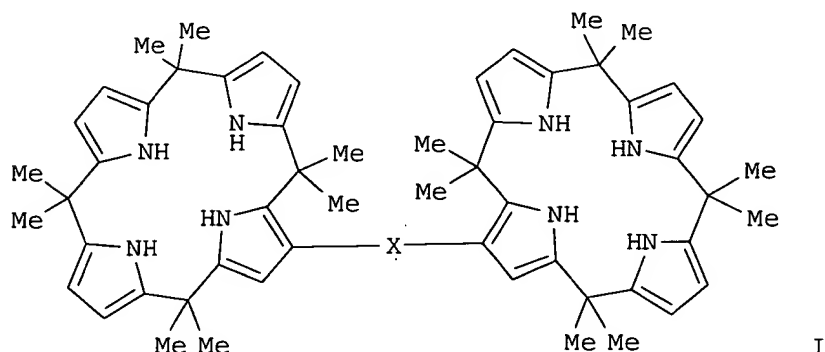
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:335221

GI



AB Calix[4]pyrrole dimers I [X = bond, p-C<sub>6</sub>H<sub>4</sub>, m-C<sub>6</sub>H<sub>4</sub>], potential hosts for anionic guests, were synthesized by a procedure involving palladium(0) catalyzed C-C bond formation. In the case of I [X = bond] a detailed study of carboxylate **anion binding** was carried out using 1H NMR spectroscopy. For isophthalate anion, a 1:1 binding stoichiometry was observed with this receptor and a much higher association constant was found than for the control monomer, octamethylcalix[4]pyrrole. These findings are ascribed to cooperative binding. Consistent with this conclusion was the finding that, for phthalate and benzoate anions, 1:2 (host:guest) binding stoichiometries and lower association consts. were recorded than with isophthalate anion. The control compound, octamethylcalix[4]pyrrole, showed a 1:1 binding stoichiometry and a much lower association constant than I [X = bond] not just with isophthalate but also



phthalate and benzoate anions.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 22 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:403700 CAPLUS  
DOCUMENT NUMBER: 133:150249  
TITLE: The complexation of halide ions by a calix[6]pyrrole  
AUTHOR(S): Cafeo, Grazia; Kohnke, Franz H.; La Torre, Giovanna  
L.; White, Andrew J. P.; Williams, David J.  
CORPORATE SOURCE: Universita di Messina, Messina, 98166, Italy  
SOURCE: Chemical Communications (Cambridge) (2000), (13),  
1207-1208  
CODEN: CHCOFS; ISSN: 1359-7345  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The X-ray crystal structures of the 1:1 complexes formed by  
calix[6]pyrrole 1b with Bun4NCl and Bun4NBr show the macrocycle to adopt  
D3d symmetry and to encapsulate the halide ions within the macrocyclic  
cavity via six N-H...X- hydrogen bonds; the  
macrocycle subtly adjusts its conformation to accommodate the differently  
sized anions; preliminary extraction expts. indicate that 1b is a dramatically  
stronger chloride ion complexing agent than its smaller calix[4]pyrrole  
analog.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 23 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:301870 CAPLUS  
DOCUMENT NUMBER: 133:37438  
TITLE: Calixarenes in analytical and separation chemistry  
AUTHOR(S): Ludwig, R.  
CORPORATE SOURCE: Radiochem. Div., Inorg. and Analyt. Chem., Institute  
of Chemistry, Freie Universitat Berlin, Berlin, 14195,  
Germany  
SOURCE: Fresenius' Journal of Analytical Chemistry (2000),  
367(2), 103-128  
CODEN: FJACES; ISSN: 0937-0633  
PUBLISHER: Springer-Verlag  
DOCUMENT TYPE: Journal; General Review  
LANGUAGE: English

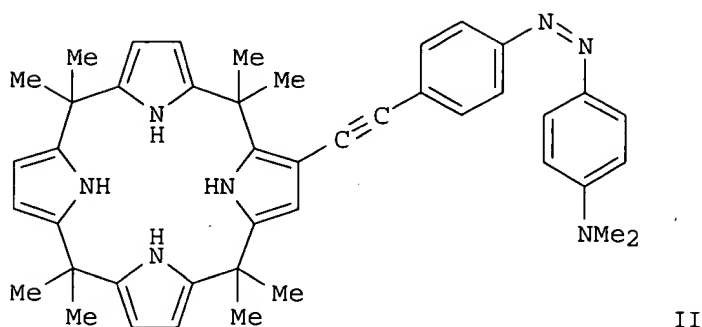
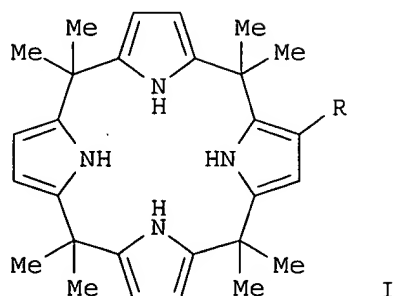
AB Discovered in the 1940's, [1n]metacyclophanes with the common name  
calix[n]arenes which is derived from the mol.'s shape enjoyed a  
remarkable interest in almost all fields of chemical since the 1980's, which  
is highlighted by several books. Over 50 reviews concerning their  
synthesis, properties and applicabilities were published; many of those  
with emphasis on organic synthesis and structural properties are cited. Of  
interest for anal. chemists are reviews on calixarenes and the  
structurally related resorcin[n]arenes (or calix[n]resorcarenes) and  
**calixpyrroles** concerning potentiometric sensors, chromo- and  
fluorophores, mol. switches, metal ion binding in solution, redox properties  
and **anion binding**. Other recent reviews deal with  
thermodn. aspects, organometallic compds., P-containing calixarenes, as well  
as mol. dynamics modeling. It is a vital field with over 200 publications  
per yr. Therefore, this article presents only selected results on  
complexation, solvent extraction and membrane transport with the emphasis on  
ion and mol. recognition which can be used for anal. purposes, without  
attempting to cover all available refs.

REFERENCE COUNT: 487 THERE ARE 487 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L17 ANSWER 24 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN



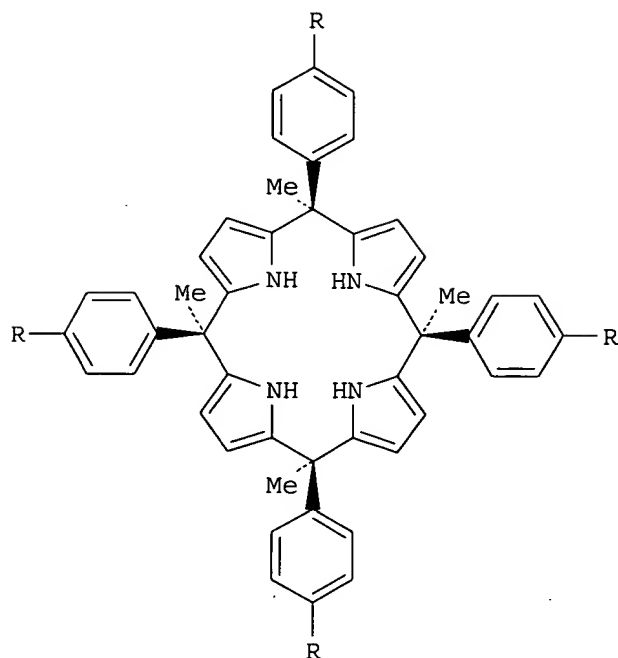
ACCESSION NUMBER: 2000:170492 CAPLUS  
 DOCUMENT NUMBER: 132:308324  
 TITLE: A "building block" approach to functionalized calix[4]pyrroles  
 AUTHOR(S): Miyajii, Hidekazu; Sato, Wataru; Sessler, Jonathan L.; Lynch, Vincent M.  
 CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, The University of Texas at Austin, Austin, TX, 78712-1167, USA  
 SOURCE: Tetrahedron Letters (2000), 41(9), 1369-1373  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 132:308324  
 GI



AB Iodocalix[4]pyrrole I (R = I) and trimethylsilylethynylcalix[4]pyrrole I (R = Me<sub>3</sub>SiC.tplbond.C) are key intermediates en route to the preparation of the alkynyl-substituted calix[4]pyrrole system I (R = HC.tplbond.C). I (R = HC.tplbond.C) in turn, provides a versatile precursor that can be used to prepare a range of arylalkynyl-functionalized calix[4]pyrroles such as II by the Sonogashira reaction of I (R = HC.tplbond.C) with appropriate aryl iodides R1I [R1 = 4-MeC<sub>6</sub>H<sub>4</sub>, 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 2,4-(O<sub>2</sub>N)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 9-phenanthrenyl, 4-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>N:N-4-C<sub>6</sub>H<sub>4</sub>] in the presence of tetrakis(triphenylphosphine)palladium(0). Significant red-shifts in the  $\lambda_{\text{max}}$  values and broadenings of the absorption peaks are seen in the UV-vis spectra of systems I [R = 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>C.tplbond.C, 2,4-(O<sub>2</sub>N)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>C.tplbond.C] upon addition of anions such as F<sup>-</sup>, Cl<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup> in CH<sub>2</sub>Cl<sub>2</sub>, a finding that leads to the suggestion that these or other analogous systems could find application as anion sensors.  
 REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



L17 ANSWER 25 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999:723546 CAPLUS  
 DOCUMENT NUMBER: 132:107806  
 TITLE: Calix[4]pyrroles Containing Deep Cavities and Fixed Walls. Synthesis, Structural Studies, and **Anion Binding** Properties of the Isomeric Products Derived from the Condensation of p-Hydroxyacetophenone and Pyrrole  
 AUTHOR(S): Anzenbacher, Pavel, Jr.; Jursikova, Karolina; Lynch, Vincent M.; Gale, Philip A.; Sessler, Jonathan L.  
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX, 78712-1167, USA  
 SOURCE: Journal of the American Chemical Society (1999), 121(47), 11020-11021  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I

AB Reaction of 4-HOC<sub>6</sub>H<sub>4</sub>Ac with pyrrole gave the calix[4]pyrrole I [R = OH] whose isomers were separated. The  $\alpha\alpha\alpha\alpha$ -,  $\alpha\alpha\alpha\beta$ -, and  $\alpha\alpha\beta\beta$ -isomers were methylated. These isomers of I [R = OH, OMe] bound F<sup>-</sup>, Cl<sup>-</sup>, and phosphate with widely varying affinities, those of I [R = OH] being higher than those of I [R = OMe]. I [R = OH] offer the opportunity to introduce secondary binding sites into these receptors.  
 REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999:574271 CAPLUS  
 DOCUMENT NUMBER: 131:327704  
 TITLE: Selective Anion Complexation by a Calix[4]pyrrole Investigated by Monte Carlo Simulations  
 AUTHOR(S): Van Hoorn, Willem P.; Jorgensen, William L.



CORPORATE SOURCE: Department of Chemistry, Yale University, New Haven,  
CT, 06520-8107, USA  
SOURCE: Journal of Organic Chemistry (1999), 64(20), 7439-7444  
CODEN: JOCEAH; ISSN: 0022-3263  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The complexation of anions by octamethylcalix[4]pyrrole 1 and 2,5-dimethylpyrrole has been investigated by energy minimizations in the gas phase and by Monte Carlo (MC) simulations in dichloromethane using the OPLS force field. In agreement with experiment, the 1,3-alternate conformation of 1, in which adjacent pyrrole rings are pointing in opposite directions, was shown to be the most stable conformation in the absence of a halide anion. The cone conformer of 1, having all pyrrole units in a parallel orientation, is not stable in the absence of a halide anion, but it is the most stable conformation upon **anion binding** due to the formation of four NH-halide hydrogen bonds. The relative free energies of binding of chloride, bromide, and iodide with the cone of 1 in dichloromethane are calculated with free energy perturbation (FEP) simulations to be in excellent agreement with experiment. However, the calcns. predict a far greater affinity for fluoride ion than was measured. This can be explained by the presence of trace amts. of water. For reference, MC/FEP calcns. were also carried out for 2,5-dimethylpyrrole, which was predicted to bind only fluoride ion, consistent with NMR expts. On the tech. side, the MC sampling efficiency of alternative internal-coordinate representations of the complexes was also considered.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 27 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:147033 CAPLUS

TITLE: **Calixpyrroles. Novel anion binding receptors**

AUTHOR(S): Sessler, Jonathan L.; Anzenbacher, Pavel, Jr.; Jursikova, Karolina; Miyaji, Hidekazu; Genge, John; Shriver, James A.; Gale, Philip A.; Kral, Vladimir

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Texas, Austin, TX, 78712, USA

SOURCE: Book of Abstracts, 217th ACS National Meeting, Anaheim, Calif., March 21-25 (1999), I&EC-206. American Chemical Society: Washington, D. C. CODEN: 67GHA6

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB The **calixpyrroles** (e.g. 1) are easy-to-make neutral **anion binding** agents and show a preference for fluoride anion over chloride anion over dihydrogen phosphate in organic media. They are also easy to functionalize. This latter property has allowed the preparation of many elaborated monomeric **calixpyrroles**, such as 2-5, as well as solid supports, such as 6, that are useful in the area of HPLC-based oligonucleotide sepn.

L17 ANSWER 28 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:409377 CAPLUS

DOCUMENT NUMBER: 129:103574

TITLE: Calix[4]pyrroles: new solid-phase HPLC supports for the separation of anions

AUTHOR(S): Sessler, Jonathan L.; Gale, Philip A.; Genge, John W.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX, 78712, USA

SOURCE: Chemistry--A European Journal (1998), 4(6), 1095-1099 CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal



LANGUAGE: English

AB The preparation of two distinct calix[4]pyrrole-modified silica gels is reported. These systems, designed to study the binding characteristics of calix[4]pyrroles with anionic and neutral substrates, also provide a new solid support for the HPLC separation of nucleotides, oligonucleotides, N-protected amino acids and perfluorinated biphenyls. Binding affinities for the interaction of anions with calix[4]pyrrole amide derivs. are also reported; these were determined from <sup>1</sup>H NMR spectroscopic analyses carried out in CD<sub>2</sub>Cl<sub>2</sub>.

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:275704 CAPLUS

DOCUMENT NUMBER: 127:17652

TITLE: Calix[4]pyrroles: C-rim substitution and tunability of **anion binding** strength

AUTHOR(S): Gale, Philip A.; Sessler, Jonathan L.; Allen, William E.; Tvermoes, Nicolai A.; Lynch, Vincent

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Chemical Communications (Cambridge) (1997), (7), 665-666

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Electron-rich and electron-deficient C-rim substituted calix[4]pyrroles are synthesized and the **anion binding** ability of these receptors is found to be dependent upon the C-rim substituents.

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:157987 CAPLUS

TITLE:  $\beta$ -Substituted calix[4]pyrroles: New chemistry at the C-rim.

AUTHOR(S): Gale, Philip A.; Allen, William E.; Genge, John; Tvermoes, Nicolai; Lynch, Vincent; Sessler, Jonathan L.

CORPORATE SOURCE: Department Chemistry and Biochemistry, University Texas, Austin, TX, 78712-1167, USA

SOURCE: Book of Abstracts, 213th ACS National Meeting, San Francisco, April 13-17 (1997), INOR-522. American Chemical Society: Washington, D. C.

CODEN: 64AOAA

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB Over the last year, calix[4]pyrroles have been shown by us to be selective **anion binding** agents. We are currently interested in adding extra functionality to the **calixpyrrole** skeleton. Two strategies have been pursued in the synthesis of  $\beta$ -substituted calix[4]pyrroles: firstly, synthesis from 3,4-disubstituted pyrroles and ketones and secondly, direct modification of the C-rim of a pre-synthesized calix[4]pyrrole. Thus, new calix[4]pyrroles (1 - 4) have been produced. The **anion binding** strengths of 1, 2 and 3 are reduced relative to their parent calix[4]pyrrole macrocycles, whereas compound 4 shows a higher affinity for anions than the  $\beta$ -free analog.

L17 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:72313 CAPLUS

DOCUMENT NUMBER: 126:144029

TITLE: **Anion binding**: self-assembly of



AUTHOR(S): polypyrrolic macrocycles  
 Sessler, Jonathan L.; Andrievsky, Andrei; Gale, Philip  
 A.; Lynch, Vincent  
 CORPORATE SOURCE: Dep. of Chemistry and Biochemistry, The University of  
 Texas at Austin, Austin, TX, 78712, USA  
 SOURCE: Angewandte Chemie, International Edition in English  
 (1997), Volume Date 1996, 35(23/24), 2782-2785  
 CODEN: ACIEAY; ISSN: 0570-0833  
 PUBLISHER: VCH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Self- and cross-assembly was examined in the sapphyrins I [R = Me, R1 = H,  
 R2 = CH<sub>2</sub>CO<sub>2</sub>H; R = CH<sub>2</sub>CO<sub>2</sub>H, R1, R2 = Me] and the **calixpyrrole** II,  
 which was prepared from Me 4-acetylbutyrate, cyclohexanone, and pyrrole.  
 Both I and II formed dimers in the gas, solution, and solid phases.  
 Cross-dimers were also obtained between I and between II and I.

REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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